



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:03 PM UTC

PDB ID : 6ZKR / pdb_00006zkr
EMDB ID : EMD-11259
Title : Native complex I, open3
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 3.50 Å(reported)
Based on initial model : 5LNK

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

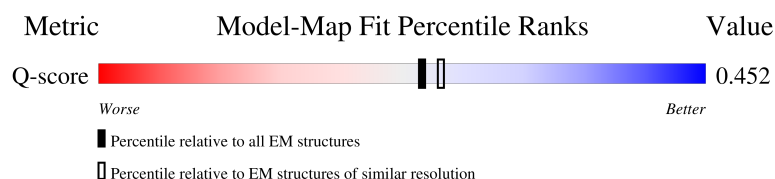
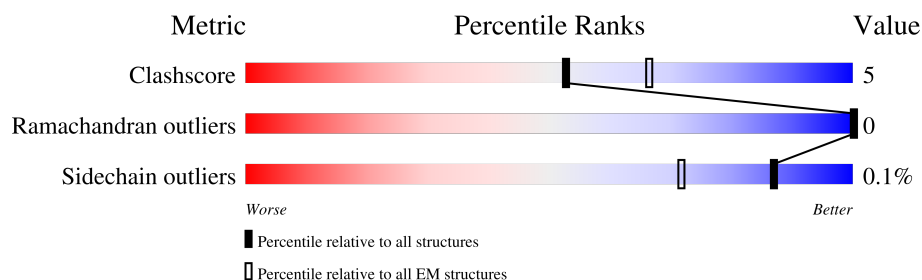
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	464	
2	2	246	
3	3	727	
4	4	463	

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Mol	Chain	Length	Quality of chain
5	5	266	
6	6	223	
7	9	217	
8	A	115	
9	H	318	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	V	141	
16	W	189	
17	X	157	
17	j	157	
18	Y	172	
19	Z	175	
20	a	109	
21	b	124	
22	c	170	
23	d	380	
24	e	99	
25	f	116	
26	g	140	
27	h	114	
28	i	145	

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Mol	Chain	Length	Quality of chain
29	k	355	
30	l	106	
31	m	84	
32	n	98	
33	o	122	
34	p	130	
35	q	144	
36	r	128	
37	s	137	
38	t	179	
39	u	108	
40	v	186	
41	w	154	
42	x	76	
43	y	58	
44	z	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	1	500	-	-	X	-
51	CDL	L	1003	X	-	-	-
51	CDL	V	204	X	-	-	-
51	CDL	Y	201	X	-	-	-
51	CDL	o	502	X	-	-	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 67353 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	421	Total	C	N	O	S	0	0
			3390	2165	581	619	25		

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	110	Total	C	N	O	S	0	0
			880	593	128	153	6		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	313	Total	C	N	O	S	0	0
			2489	1680	379	411	19		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1273	856	182	222	13		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4806	3187	746	829	44		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 15 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
17	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 19 is a protein called Mitochondrial complex I, PDSW subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 20 is a protein called Mitochondrial complex I, 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 21 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 25 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 27 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 35 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 36 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 41 is a protein called Mitochondrial complex I, ESSS subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 42 is a protein called Mitochondrial complex I, KFYI subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	x	49	Total	C	N	O	0	0
			412	271	70	71		

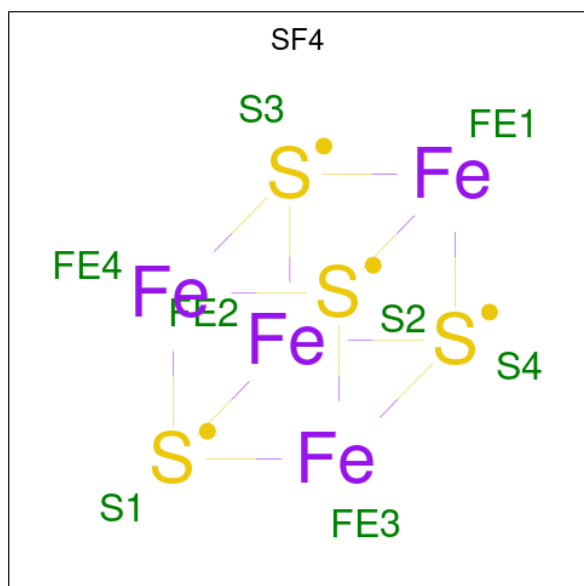
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	y	50	Total	C	N	O	0	0
			436	287	77	72		

- Molecule 44 is a protein called Mitochondrial complex I, MWFE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	6	1	Total	Fe	S	0
			8	4	4	

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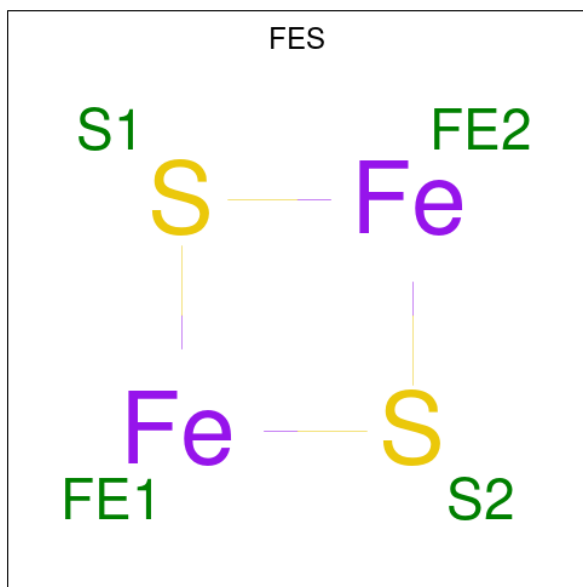
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

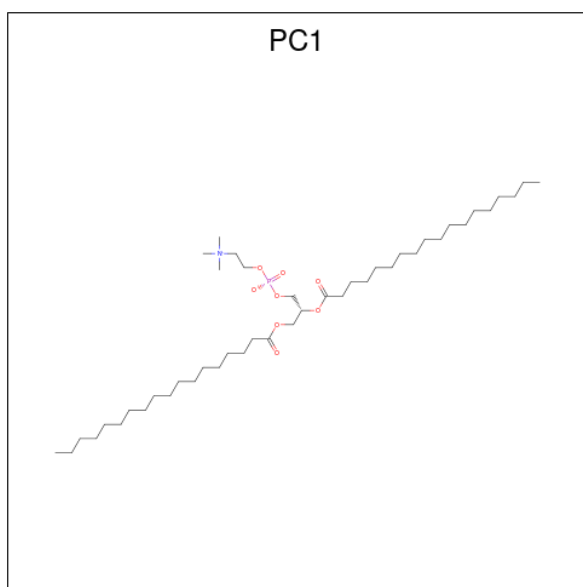


Mol	Chain	Residues	Atoms			AltConf
47	2	1	Total	Fe	S	0
			4	2	2	
47	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is POTASSIUM ION (CCD ID: K) (formula: K).

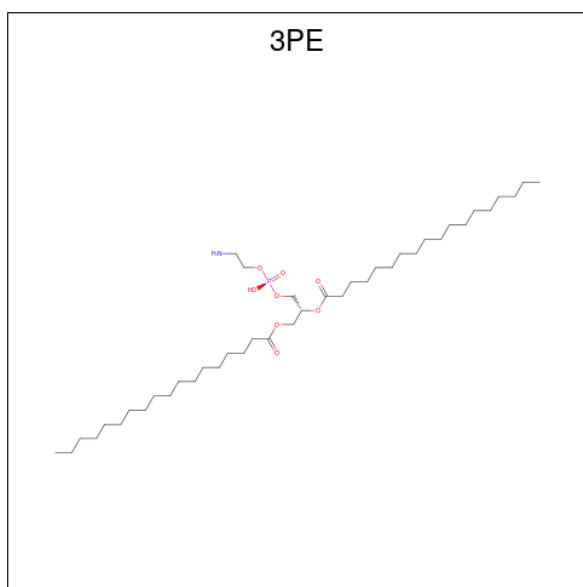
Mol	Chain	Residues	Atoms		AltConf
48	3	1	Total	K	0
			1	1	

- Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



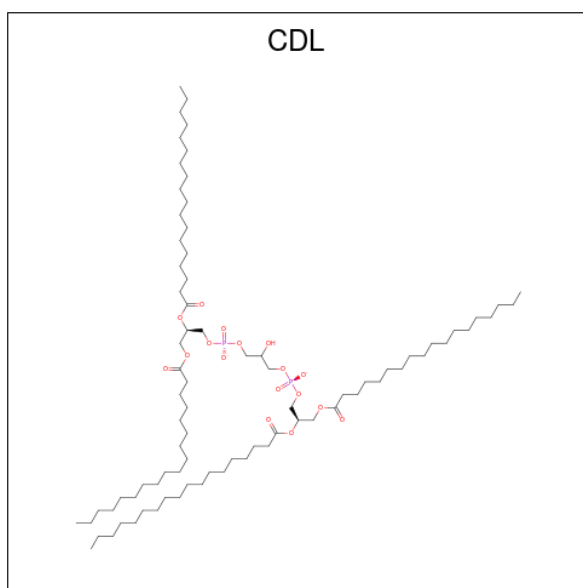
Mol	Chain	Residues	Atoms					AltConf
49	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
49	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
49	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
49	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
49	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
49	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



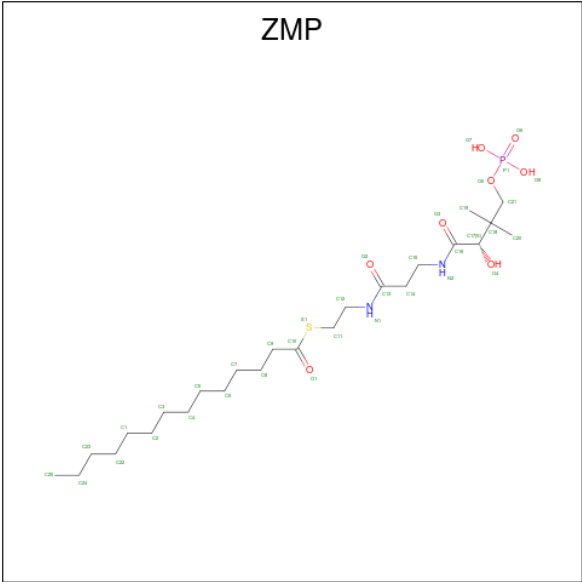
Mol	Chain	Residues	Atoms					AltConf
50	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	K	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
50	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
50	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	o	1	Total	C	N	O	P	0
			31	21	1	8	1	
50	p	1	Total	C	O	P		0
			27	18	8	1		

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
51	L	1	Total	C	O	P	0
			100	81	17	2	
51	M	1	Total	C	O	P	0
			90	71	17	2	
51	V	1	Total	C	O	P	0
			94	75	17	2	
51	V	1	Total	C	O	P	0
			85	66	17	2	
51	W	1	Total	C	O	P	0
			100	81	17	2	
51	Y	1	Total	C	O	P	0
			100	81	17	2	
51	o	1	Total	C	O	P	0
			75	56	17	2	
51	z	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 52 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

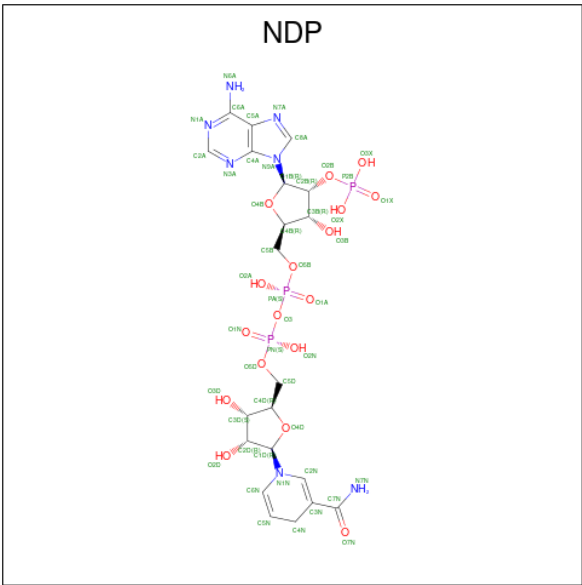


Mol	Chain	Residues	Atoms					AltConf
52	X	1	Total	C	N	O	P	S
			31	20	2	7	1	1
52	g	1	Total	C	N	O	P	S
			34	23	2	7	1	1

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

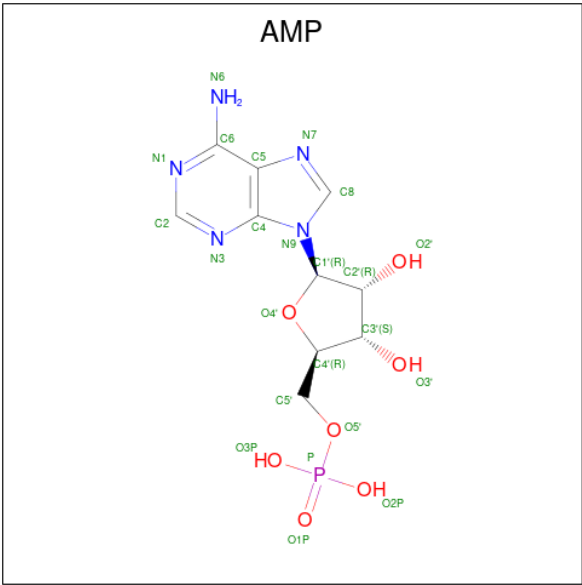
Mol	Chain	Residues	Atoms		AltConf
53	b	1	Total	Zn	0
			1	1	

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



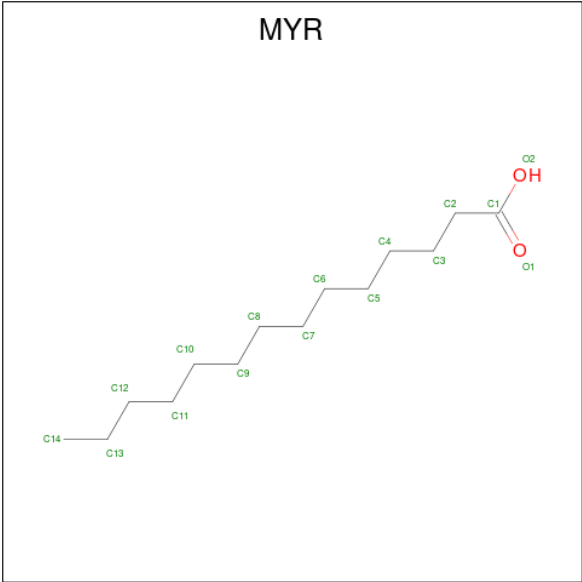
Mol	Chain	Residues	Atoms					AltConf
54	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 55 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					AltConf
55	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 56 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).

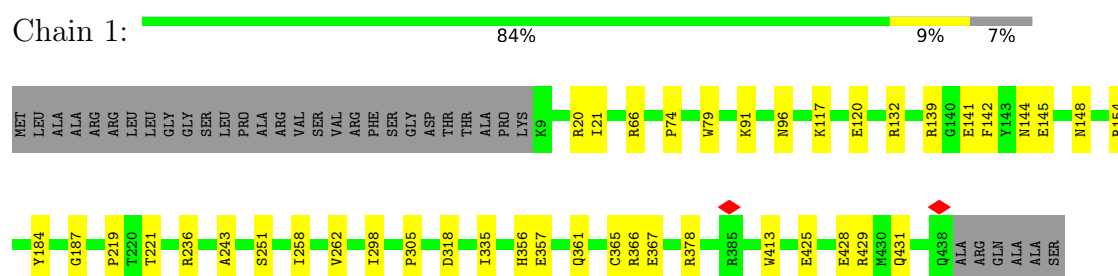


Mol	Chain	Residues	Atoms			AltConf
56	s	1	Total	C	O	0
			15	14	1	

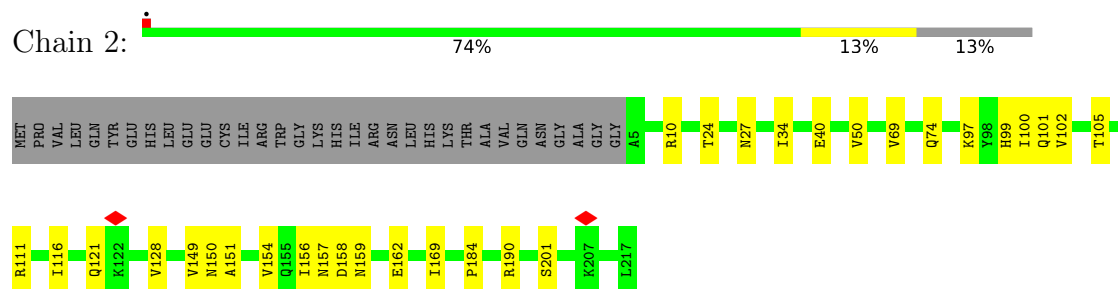
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

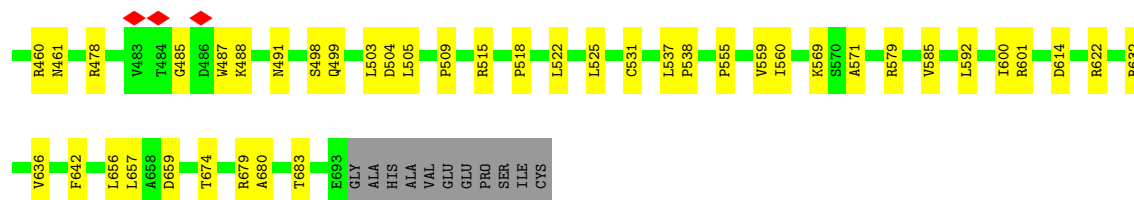


- Molecule 2: Mitochondrial complex I, 24 kDa subunit

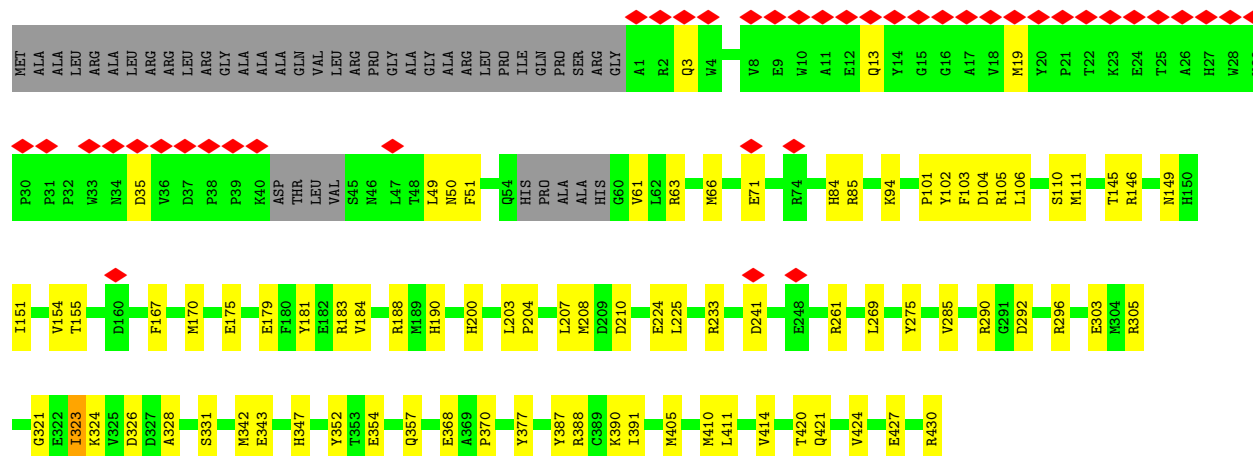
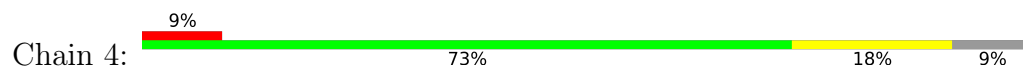


- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

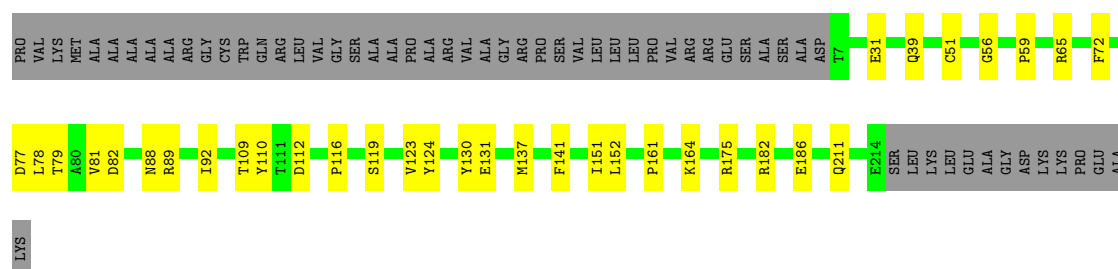




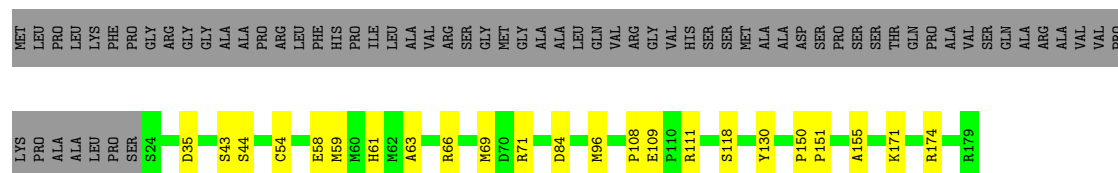
• Molecule 4: Mitochondrial complex I, 49 kDa subunit



• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

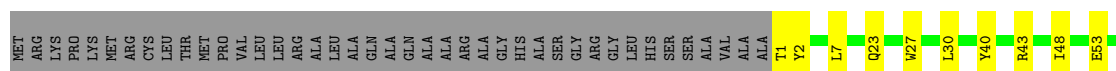


• Molecule 6: Mitochondrial complex I, PSST subunit

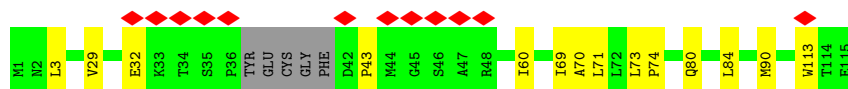
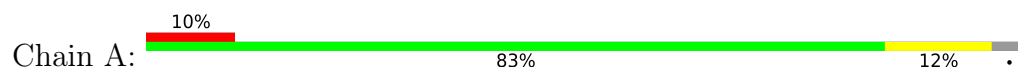


• Molecule 7: Mitochondrial complex I, TYKY subunit

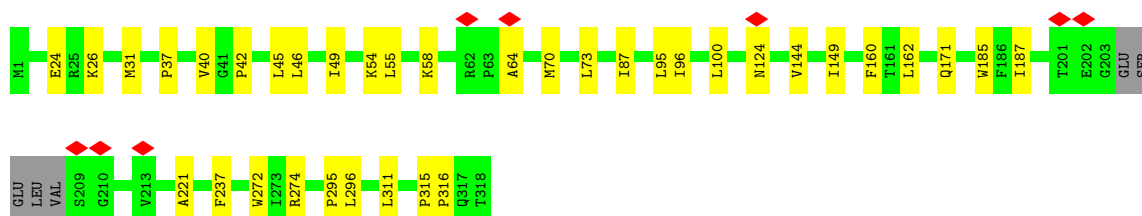
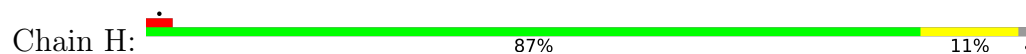




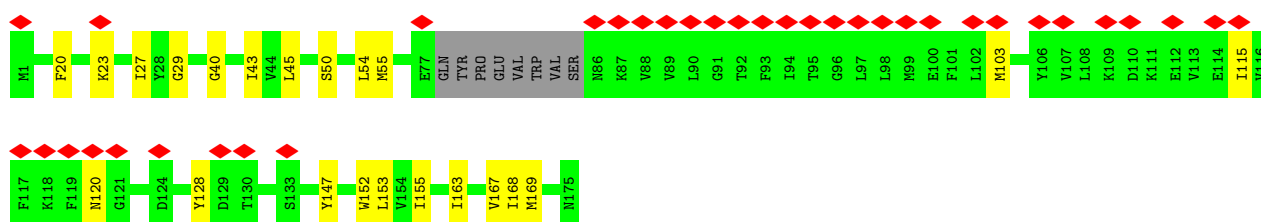
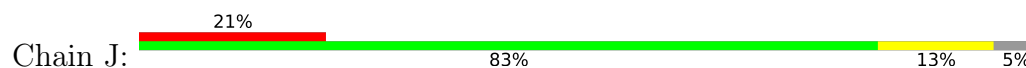
- Molecule 8: NADH-ubiquinone oxidoreductase chain 3



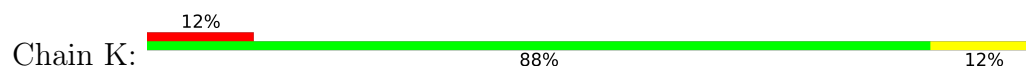
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1



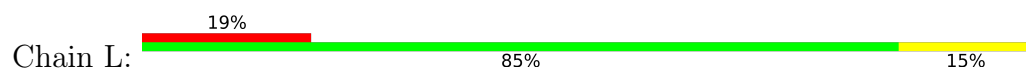
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

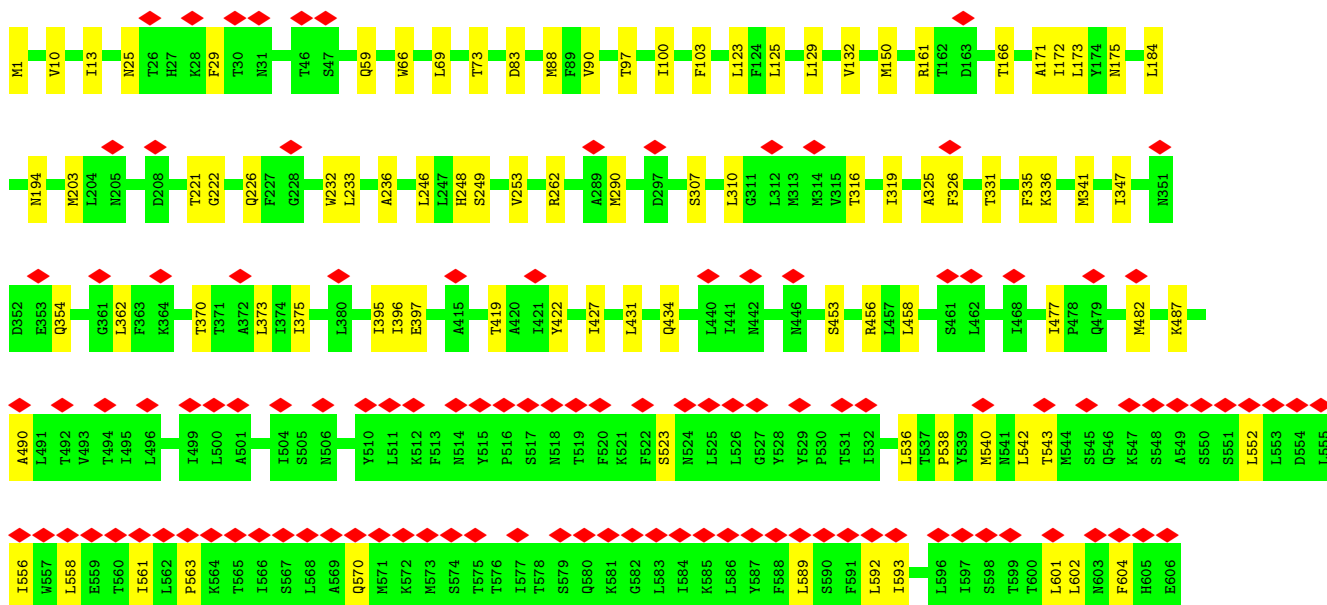


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

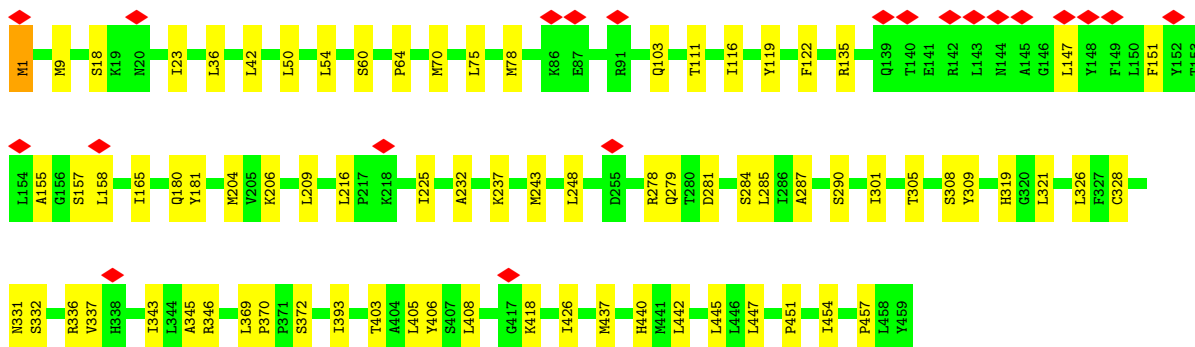
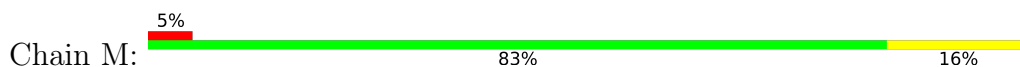


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

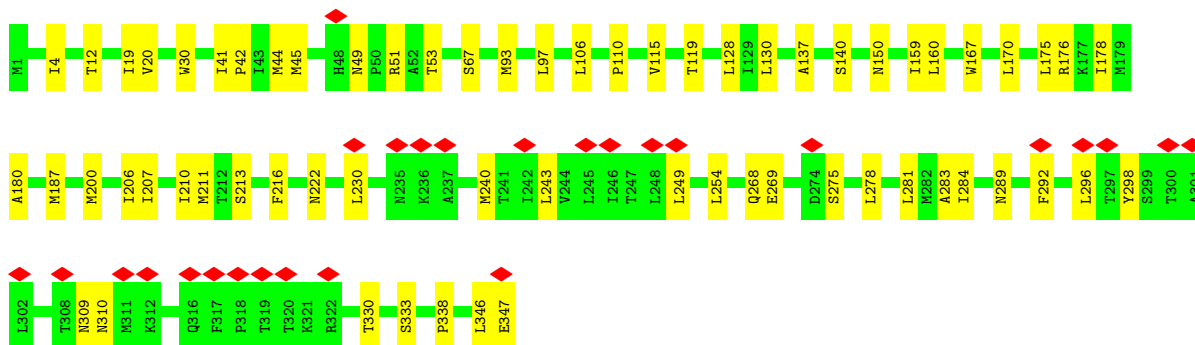
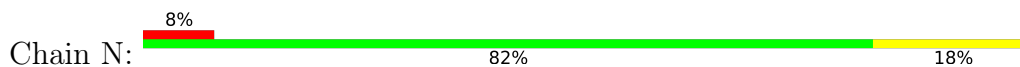




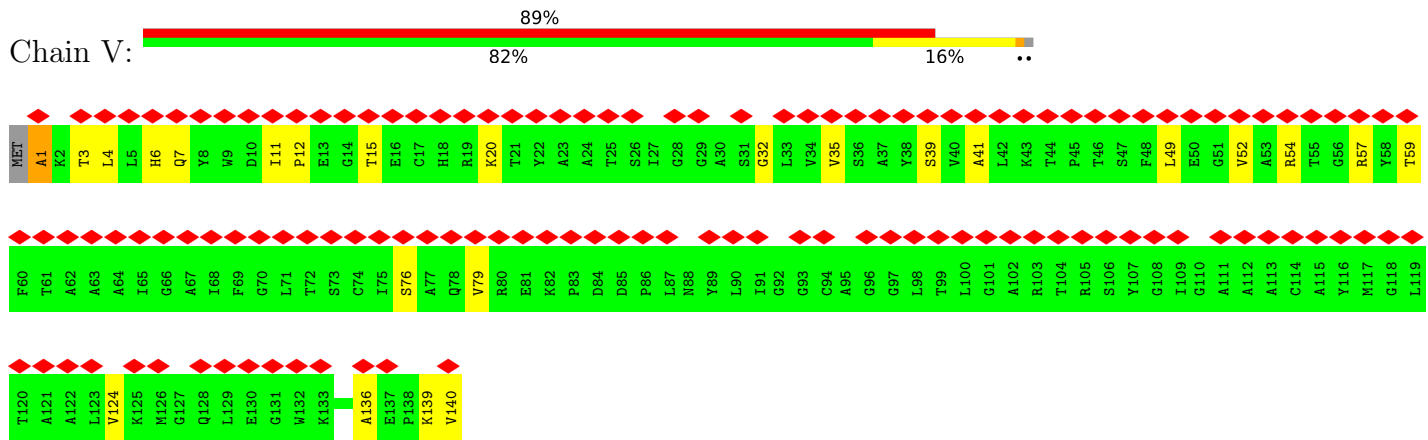
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



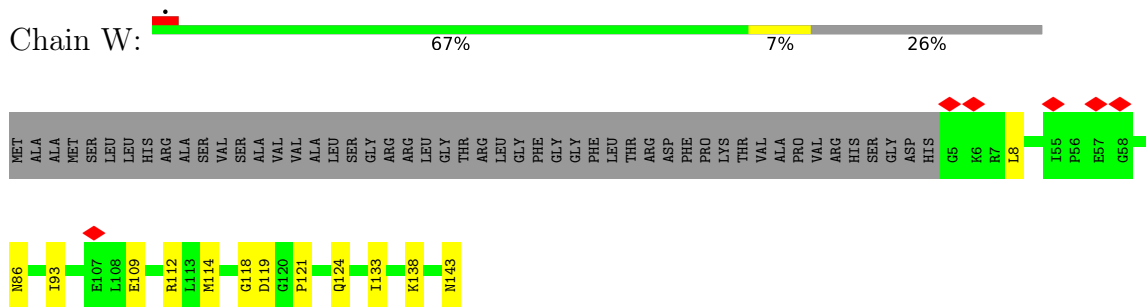
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



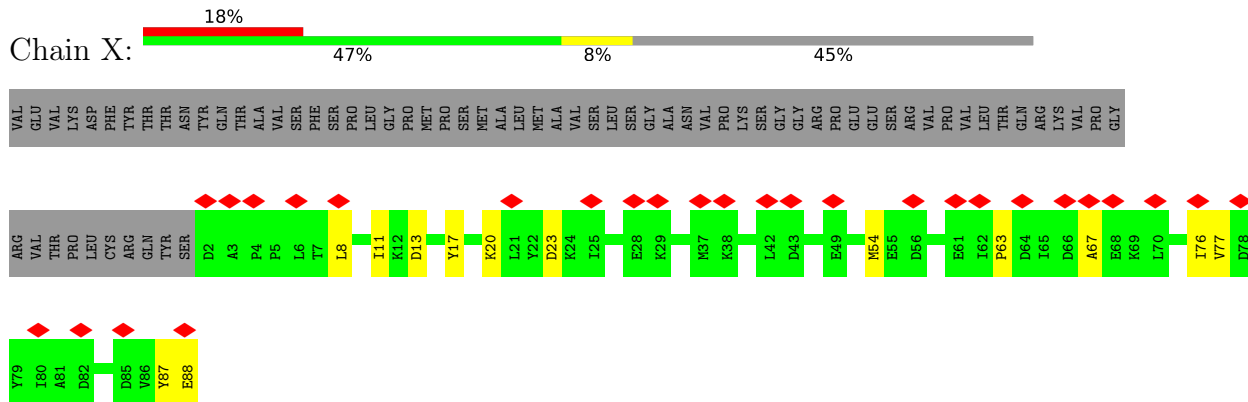
• Molecule 15: Mitochondrial complex I, B14.7 subunit



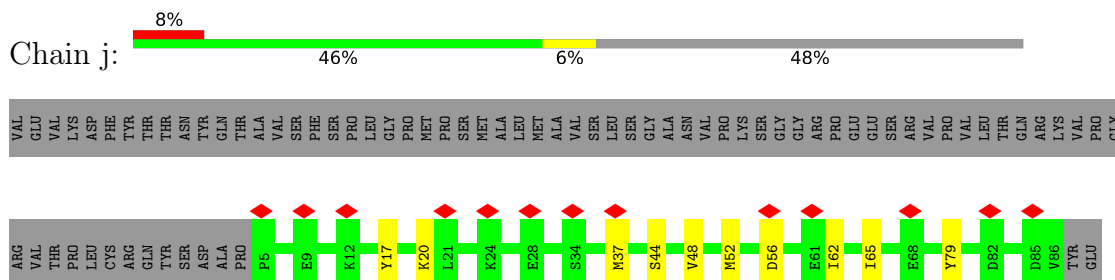
- Molecule 16: NADH:ubiquinone oxidoreductase subunit B5



- Molecule 17: Acyl carrier protein



- Molecule 17: Acyl carrier protein



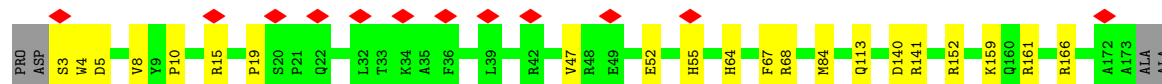
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:  86% 13%



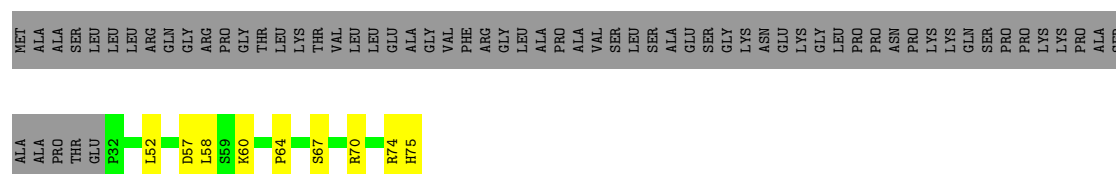
- Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z:  7% 86% 12%



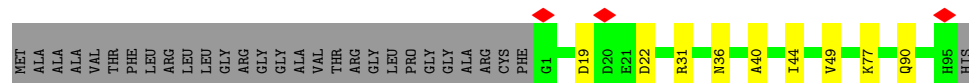
- Molecule 20: Mitochondrial complex I, 10 kDa subunit

Chain a:  32% 8% 60%



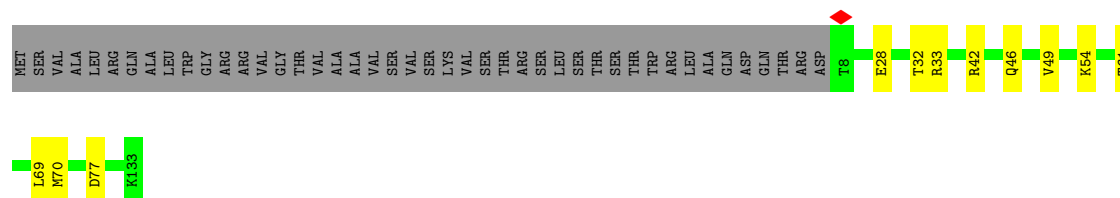
- Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b:  69% 7% 23%



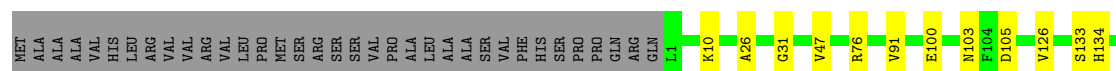
- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

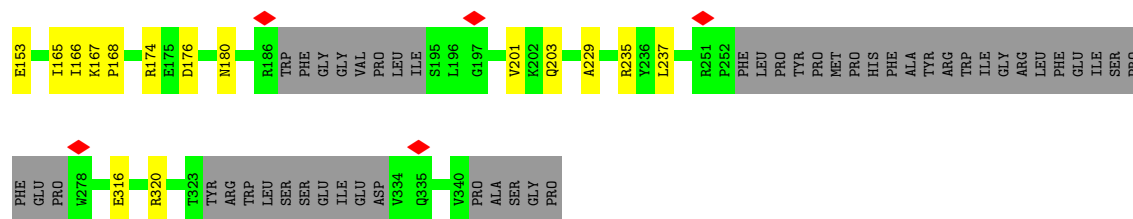
Chain c:  68% 6% 26%



- Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

Chain d:  71% 7% 22%

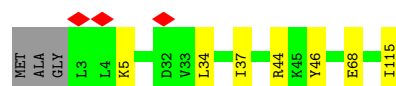
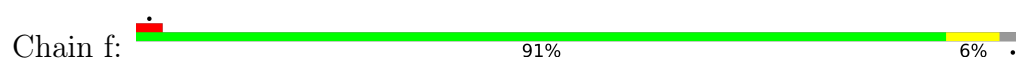




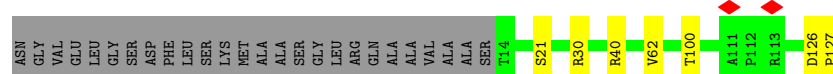
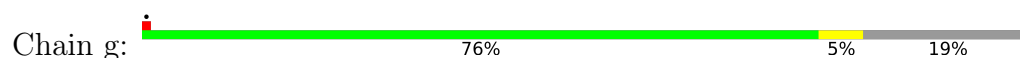
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 25: Mitochondrial complex I, B13 subunit



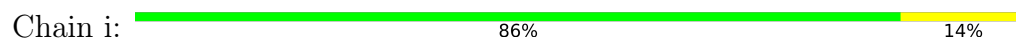
- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6



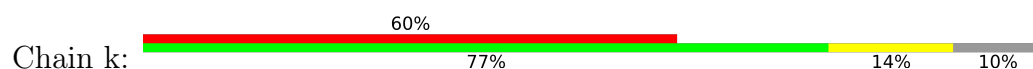
- Molecule 27: Mitochondrial complex I, B14.5a subunit

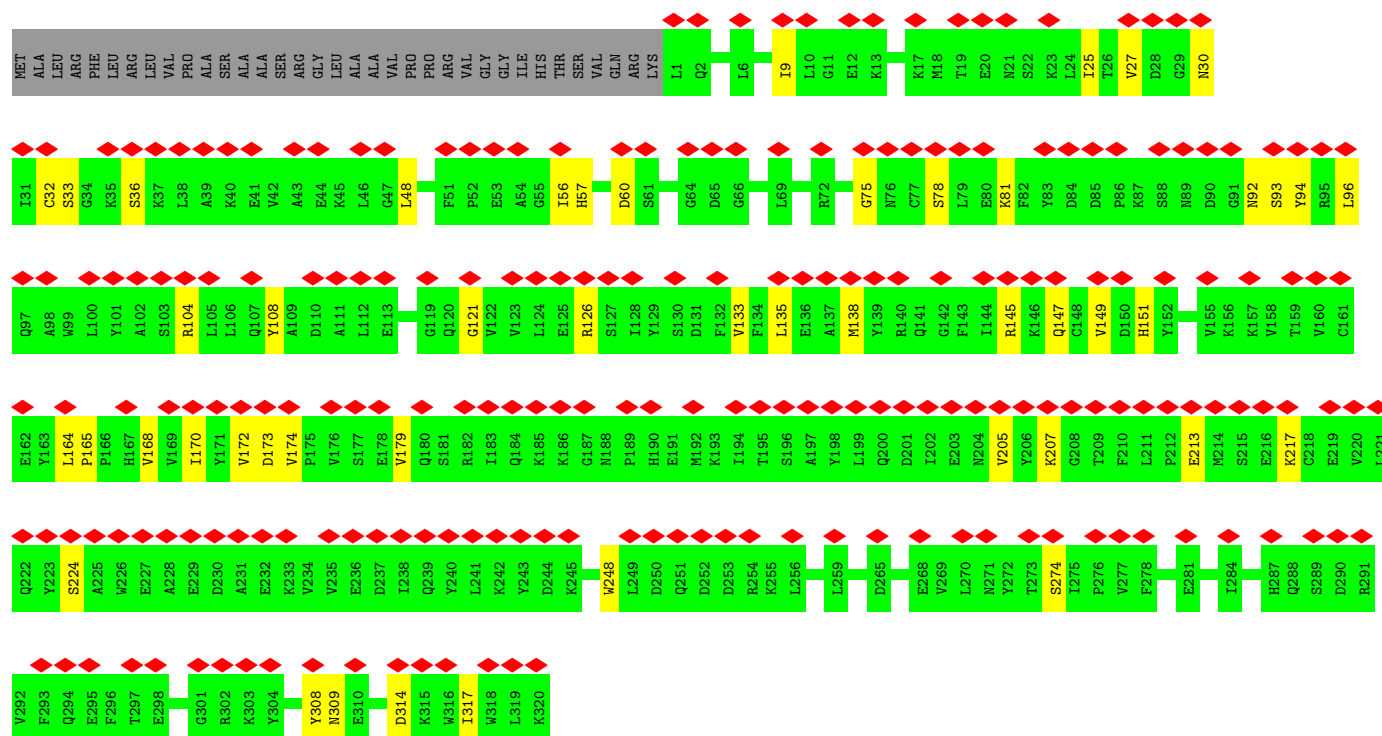


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

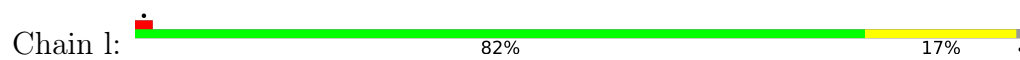


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

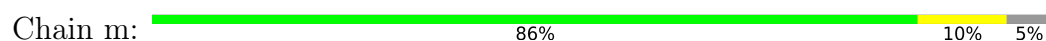




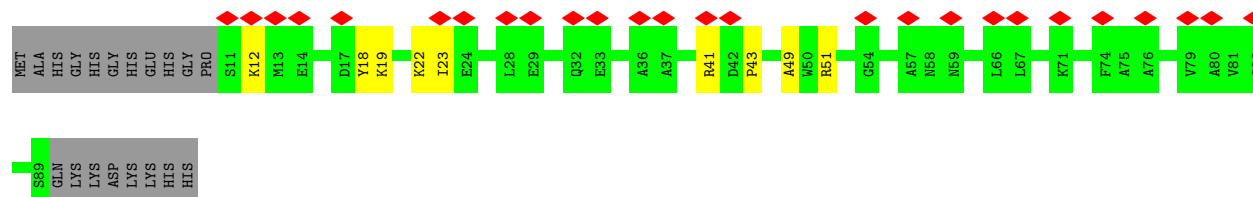
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



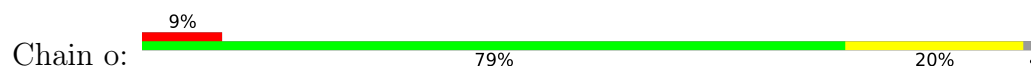
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

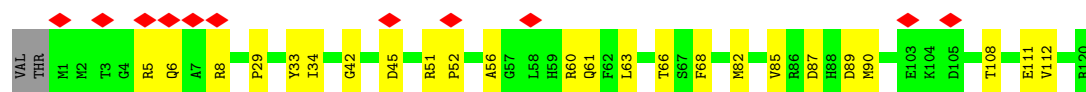


- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

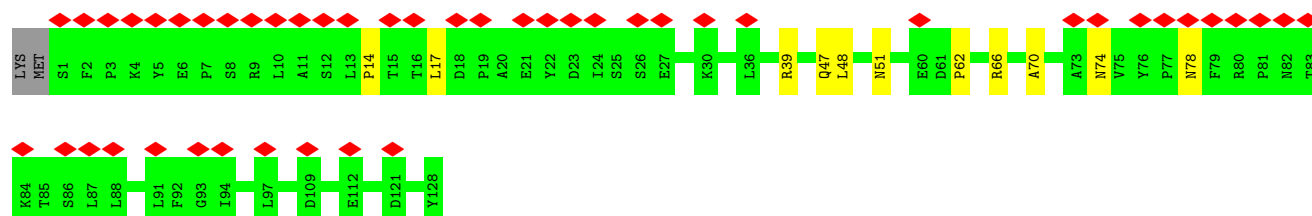
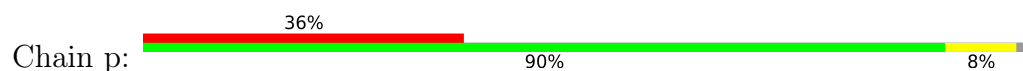


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

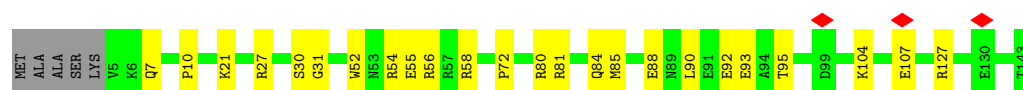
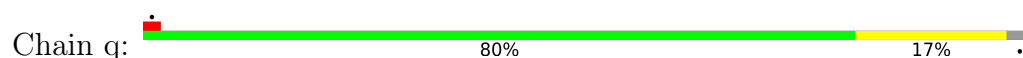




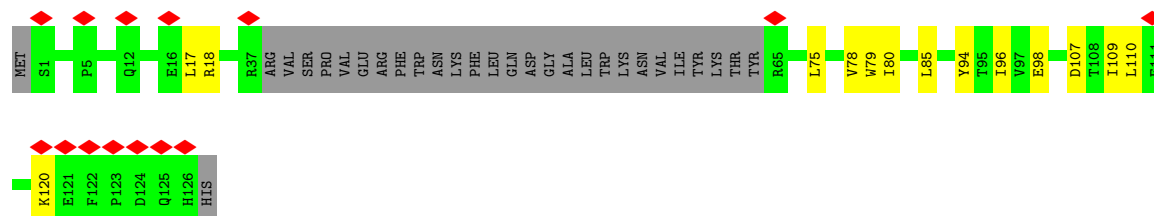
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



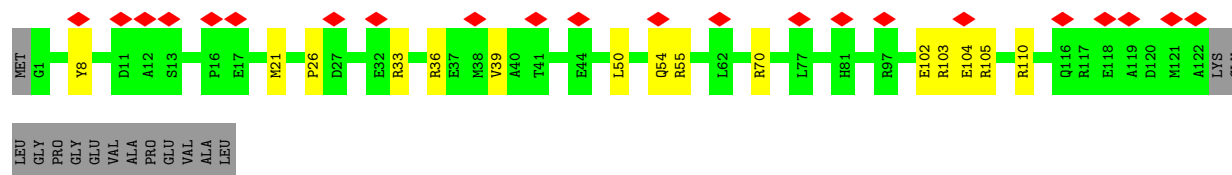
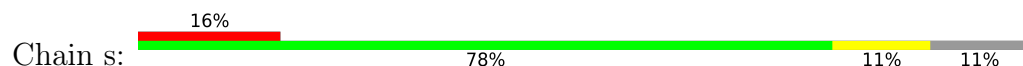
- Molecule 35: Mitochondrial complex I, B16.6 subunit



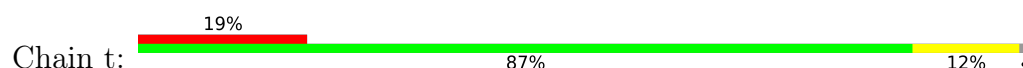
- Molecule 36: Mitochondrial complex I, B17 subunit

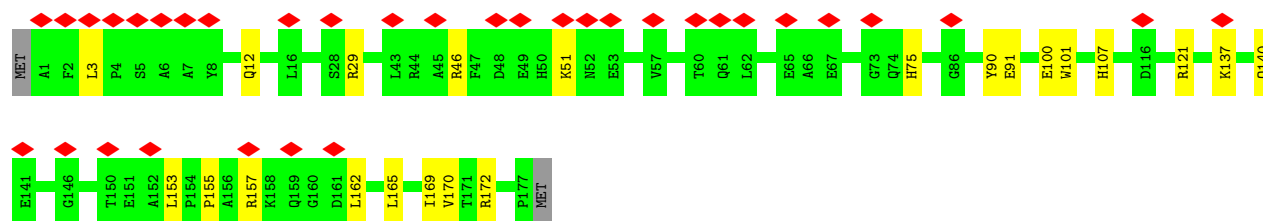


- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

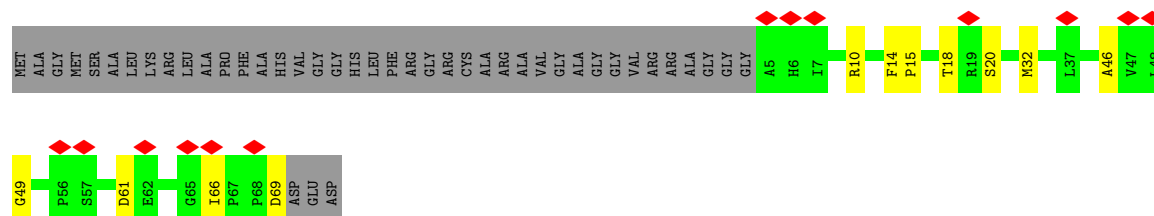


- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

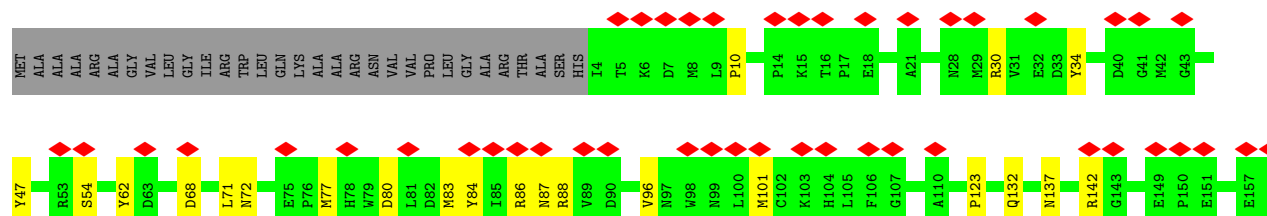




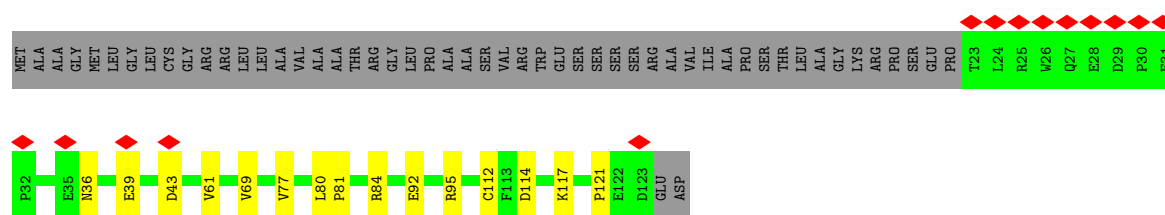
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2



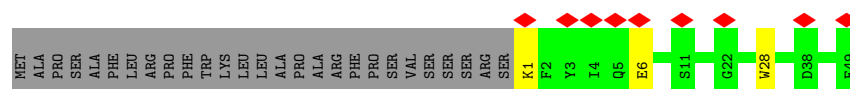
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 41: Mitochondrial complex I, ESSS subunit



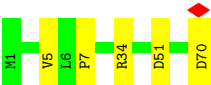
- Molecule 42: Mitochondrial complex I, KFYI subunit



- Molecule 43: Mitochondrial complex I, MNLL subunit



● Molecule 44: Mitochondrial complex I, MWFE subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20316	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	170.98, 195.05, 291.33	wwPDB
Map dimensions	351, 235, 206	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, NDP, SF4, AYA, ZMP, FMN, FES, 3PE, K, PC1, CDL, FME, AMP, ZN, MYR, 2MR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.34	0/3386	0.56	0/4575
2	2	0.33	0/1695	0.58	0/2306
3	3	0.36	0/5362	0.56	2/7266 (0.0%)
4	4	0.39	0/3463	0.56	0/4687
5	5	0.36	0/1776	0.53	0/2417
6	6	0.41	0/1278	0.56	0/1728
7	9	0.44	0/1445	0.59	0/1956
8	A	0.32	0/902	0.63	0/1234
9	H	0.38	0/2563	0.63	0/3505
10	J	0.32	0/1302	0.56	0/1760
11	K	0.34	0/749	0.59	0/1014
12	L	0.28	0/4924	0.58	0/6698
13	M	0.33	0/3731	0.57	0/5085
14	N	0.35	0/2787	0.59	0/3795
15	V	0.23	0/1041	0.48	0/1412
16	W	0.27	0/1188	0.49	0/1607
17	X	0.22	0/713	0.51	0/963
17	j	0.21	0/670	0.49	0/902
18	Y	0.28	0/1440	0.52	0/1942
19	Z	0.25	0/1475	0.48	0/1989
20	a	0.25	0/383	0.45	0/518
21	b	0.30	0/749	0.49	0/1009
22	c	0.34	0/1047	0.47	0/1415
23	d	0.30	0/2424	0.48	0/3276
24	e	0.26	0/702	0.49	0/945
25	f	0.27	0/937	0.52	0/1271
26	g	0.29	0/993	0.50	0/1336
27	h	0.32	0/779	0.53	0/1053
28	i	0.32	0/1250	0.47	0/1698
29	k	0.20	0/2646	0.45	0/3579
30	l	0.30	0/896	0.53	0/1200
31	m	0.27	0/647	0.51	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	n	0.19	0/653	0.44	0/882
33	o	0.25	0/1035	0.45	0/1398
34	p	0.21	0/1085	0.48	0/1467
35	q	0.29	0/1171	0.52	0/1579
36	r	0.24	0/874	0.54	0/1188
37	s	0.21	0/1072	0.50	0/1436
38	t	0.22	0/1573	0.53	0/2130
39	u	0.21	0/590	0.50	0/810
40	v	0.21	0/1361	0.50	0/1861
41	w	0.25	0/872	0.51	0/1185
42	x	0.20	0/425	0.44	0/576
43	y	0.24	0/449	0.49	0/605
44	z	0.35	0/591	0.53	0/795
All	All	0.31	0/67094	0.54	2/90943 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
3	3	0	1
4	4	0	1
8	A	0	2
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	366	THR	CA-C-N	5.97	132.94	121.54
3	3	366	THR	C-N-CA	5.97	132.94	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	158	ASP	Peptide
3	3	259	ASN	Peptide
4	4	275	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	A	113	TRP	Peptide
8	A	29	VAL	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3312	0	3269	26	0
2	2	1655	0	1668	19	0
3	3	5275	0	5300	82	0
4	4	3390	0	3333	60	0
5	5	1726	0	1676	21	0
6	6	1247	0	1259	19	0
7	9	1414	0	1371	30	0
8	A	880	0	920	14	0
9	H	2489	0	2603	28	0
10	J	1273	0	1300	21	0
11	K	749	0	793	10	0
12	L	4806	0	4945	67	0
13	M	3647	0	3849	59	0
14	N	2723	0	2930	44	0
15	V	1028	0	1036	19	0
16	W	1155	0	1177	12	0
17	X	701	0	692	10	0
17	j	660	0	663	7	0
18	Y	1403	0	1392	21	0
19	Z	1441	0	1419	17	0
20	a	371	0	344	7	0
21	b	737	0	710	7	0
22	c	1024	0	1023	11	0
23	d	2372	0	2407	16	0
24	e	691	0	706	13	0
25	f	917	0	958	5	0
26	g	969	0	980	6	0
27	h	769	0	780	9	0
28	i	1209	0	1182	16	0
29	k	2596	0	2559	28	0
30	l	874	0	869	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	m	626	0	635	6	0
32	n	634	0	616	7	0
33	o	1004	0	995	17	0
34	p	1059	0	1062	9	0
35	q	1142	0	1137	21	0
36	r	846	0	864	12	0
37	s	1047	0	1015	11	0
38	t	1520	0	1477	18	0
39	u	563	0	509	8	0
40	v	1307	0	1207	19	0
41	w	846	0	792	14	0
42	x	412	0	411	2	0
43	y	436	0	437	6	0
44	z	576	0	570	6	0
45	1	8	0	0	2	0
45	3	16	0	0	1	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	0	0
47	2	4	0	0	1	0
47	3	4	0	0	0	0
48	3	1	0	0	0	0
49	6	46	0	69	0	0
49	9	54	0	88	2	0
49	A	37	0	48	2	0
49	L	54	0	88	5	0
49	M	108	0	176	8	0
50	6	51	0	82	3	0
50	A	51	0	82	1	0
50	H	51	0	82	3	0
50	K	40	0	54	1	0
50	L	82	0	118	2	0
50	M	84	0	119	4	0
50	N	51	0	82	0	0
50	V	72	0	92	4	0
50	i	51	0	82	1	0
50	o	31	0	36	0	0
50	p	27	0	27	0	0
51	L	100	0	156	11	0
51	M	90	0	133	3	0
51	V	179	0	261	9	0
51	W	100	0	156	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Y	100	0	156	10	0
51	o	75	0	97	2	0
51	z	58	0	60	0	0
52	X	31	0	34	4	0
52	g	34	0	40	2	0
53	b	1	0	0	0	0
54	d	48	0	26	0	0
55	k	23	0	12	0	0
56	s	15	0	27	0	0
All	All	67353	0	68342	713	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (713) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:i:26:VAL:O	28:i:30:ALA:HB3	1.88	0.73
4:4:50:ASN:HD21	4:4:63:ARG:HH21	1.40	0.67
51:Y:201:CDL:H312	33:o:29:PRO:HB3	1.75	0.67
51:L:1003:CDL:H162	51:L:1003:CDL:H372	1.77	0.66
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.79	0.65
12:L:602:LEU:HD21	51:V:203:CDL:H432	1.80	0.64
34:p:62:PRO:O	34:p:66:ARG:HB2	1.97	0.64
10:J:120:ASN:ND2	30:l:72:MET:SD	2.70	0.64
4:4:175:GLU:OE2	4:4:188:ARG:NH1	2.30	0.64
12:L:100:ILE:HG21	12:L:246:LEU:HB2	1.80	0.64
12:L:593:ILE:HD12	15:V:41:ALA:HB2	1.79	0.64
4:4:405:MET:SD	4:4:421:GLN:NE2	2.68	0.63
30:l:96:HIS:HA	30:l:101:GLU:HG2	1.79	0.63
9:H:26:LYS:HB3	44:z:5:VAL:HG12	1.81	0.63
13:M:418:LYS:HB3	40:v:68:ASP:HB3	1.81	0.63
24:e:13:LEU:HD22	24:e:16:ARG:HH22	1.63	0.63
29:k:81:LYS:HD2	29:k:92:ASN:HD22	1.62	0.63
1:1:132:ARG:NH2	20:a:64:PRO:O	2.31	0.62
7:9:43:ARG:HG2	27:h:11:ARG:HD2	1.82	0.62
3:3:127:ARG:NH2	4:4:326:ASP:O	2.33	0.62
14:N:106:LEU:HD22	14:N:187:MET:HE2	1.82	0.62
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.64	0.62
9:H:64:ALA:O	9:H:124:ASN:ND2	2.33	0.61
35:q:81:ARG:NH1	35:q:85:MET:SD	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:161:ARG:NH2	38:t:90:TYR:O	2.33	0.61
18:Y:89:ASP:OD2	44:z:34:ARG:NH1	2.34	0.61
8:A:32:GLU:HB3	23:d:320:ARG:HH12	1.64	0.61
24:e:19:ARG:HB2	24:e:65:TRP:HB2	1.80	0.61
14:N:45:MET:HE3	14:N:53:THR:HG22	1.81	0.61
3:3:632:ARG:HH12	24:e:59:ASP:H	1.49	0.61
18:Y:165:ARG:NH1	33:o:87:ASP:OD1	2.34	0.61
19:Z:15:ARG:HB3	36:r:109:ILE:HD12	1.83	0.61
5:5:65:ARG:NH1	5:5:123:VAL:O	2.34	0.60
23:d:174:ARG:NH2	23:d:316:GLU:OE2	2.34	0.60
37:s:50:LEU:HB2	37:s:55:ARG:HE	1.65	0.60
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.82	0.60
14:N:178:ILE:HD13	14:N:296:LEU:HD11	1.83	0.60
24:e:23:CYS:SG	24:e:24:GLN:N	2.74	0.60
10:J:20:PHE:HB2	10:J:29:GLY:HA2	1.82	0.60
17:X:8:LEU:H	17:X:87:TYR:HE2	1.50	0.60
2:2:105:THR:OG1	47:2:300:FES:S2	2.60	0.60
7:9:158:GLY:O	7:9:162:GLU:HB2	2.02	0.60
51:W:201:CDL:H341	51:W:201:CDL:H511	1.84	0.60
14:N:170:LEU:HD23	14:N:292:PHE:HB3	1.84	0.59
24:e:64:LEU:HB3	24:e:76:VAL:HB	1.85	0.59
25:f:37:ILE:O	25:f:44:ARG:NH1	2.35	0.59
29:k:173:ASP:HB2	29:k:224:SER:HA	1.82	0.59
6:6:108:PRO:HB2	9:H:58:LYS:HD2	1.83	0.59
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.36	0.59
37:s:26:PRO:O	37:s:33:ARG:NH1	2.34	0.59
2:2:10:ARG:NH2	3:3:138:GLU:OE2	2.36	0.59
9:H:149:ILE:HG21	9:H:185:TRP:HB2	1.85	0.59
51:Y:201:CDL:H641	51:Y:201:CDL:H872	1.84	0.59
19:Z:19:PRO:HD3	36:r:110:LEU:HD11	1.83	0.59
2:2:100:ILE:HG12	2:2:156:ILE:HG12	1.85	0.59
40:v:80:ASP:HB3	40:v:83:MET:HB3	1.85	0.59
3:3:460:ARG:NH1	3:3:659:ASP:O	2.36	0.58
12:L:232:TRP:O	12:L:236:ALA:HB2	2.03	0.58
4:4:324:LYS:HD3	4:4:331:SER:HB3	1.84	0.58
13:M:343:ILE:O	13:M:346:ARG:NH1	2.36	0.58
29:k:145:ARG:NH1	29:k:147:GLN:OE1	2.37	0.58
20:a:57:ASP:OD1	20:a:60:LYS:NZ	2.36	0.58
1:1:21:ILE:O	1:1:117:LYS:NZ	2.35	0.58
7:9:92:ILE:HG12	7:9:111:ILE:HG12	1.85	0.58
31:m:83:LEU:HD13	35:q:54:ARG:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:632:ARG:NH1	24:e:57:CYS:SG	2.77	0.58
3:3:118:ASP:OD2	22:c:46:GLN:NE2	2.37	0.58
4:4:321:GLY:O	35:q:7:GLN:NE2	2.37	0.58
14:N:207:ILE:HG22	14:N:211:MET:HE2	1.86	0.58
34:p:48:LEU:HD23	38:t:165:LEU:HD21	1.85	0.58
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.85	0.57
4:4:241:ASP:OD1	4:4:290:ARG:NH2	2.36	0.57
34:p:39:ARG:NH2	38:t:3:LEU:O	2.38	0.57
6:6:118:SER:N	45:6:201:SF4:S4	2.77	0.57
20:a:70:ARG:NH1	20:a:75:HIS:O	2.38	0.57
37:s:33:ARG:HH12	37:s:103:ARG:HH22	1.51	0.57
40:v:68:ASP:HA	40:v:86:ARG:HH21	1.70	0.57
12:L:249:SER:HB2	12:L:336:LYS:HG3	1.86	0.57
3:3:276:ARG:HA	28:i:135:GLN:HB2	1.86	0.57
3:3:396:ARG:NH1	3:3:416:THR:O	2.38	0.57
4:4:261:ARG:NH2	4:4:303:GLU:OE2	2.38	0.57
6:6:71:ARG:HA	9:H:37:PRO:HA	1.87	0.57
51:Y:201:CDL:H572	33:o:33:TYR:HB2	1.85	0.57
39:u:10:ARG:NH1	39:u:14:PHE:O	2.37	0.57
14:N:281:LEU:HD11	50:V:202:3PE:H3A1	1.87	0.56
3:3:122:MET:O	27:h:60:ARG:NH2	2.38	0.56
10:J:23:LYS:O	11:K:23:ARG:NH1	2.38	0.56
4:4:377:TYR:HB3	4:4:390:LYS:HB3	1.87	0.56
12:L:175:ASN:ND2	12:L:222:GLY:O	2.38	0.56
36:r:107:ASP:OD2	37:s:70:ARG:NH2	2.38	0.56
12:L:552:LEU:HA	12:L:556:ILE:HD12	1.88	0.56
51:L:1003:CDL:HA61	51:L:1003:CDL:HA22	1.88	0.56
18:Y:35:CYS:O	18:Y:39:ASN:ND2	2.39	0.56
51:L:1003:CDL:H431	49:M:503:PC1:H291	1.87	0.56
17:X:13:ASP:OD2	32:n:12:LYS:NZ	2.38	0.56
34:p:47:GLN:HG3	38:t:165:LEU:HD13	1.87	0.56
14:N:243:LEU:HD22	14:N:330:THR:HG21	1.86	0.56
18:Y:63:ASN:OD1	35:q:80:ARG:NH2	2.38	0.56
3:3:47:SER:O	3:3:161:ARG:NH1	2.39	0.56
1:1:356:HIS:O	3:3:177:ARG:NH2	2.39	0.55
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.88	0.55
19:Z:68:ARG:NH1	43:y:43:LEU:O	2.37	0.55
3:3:221:GLU:OE2	3:3:243:ARG:NH1	2.39	0.55
15:V:140:VAL:HG12	16:W:112:ARG:HB2	1.87	0.55
29:k:173:ASP:OD1	29:k:207:LYS:NZ	2.40	0.55
3:3:261:GLU:OE1	22:c:42:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:109:GLU:OE2	16:W:112:ARG:NH2	2.40	0.55
23:d:203:GLN:HB3	23:d:235:ARG:HA	1.87	0.55
3:3:461:ASN:HB2	3:3:657:LEU:HD11	1.88	0.55
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.88	0.55
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.34	0.55
6:6:71:ARG:NH2	7:9:48:ILE:O	2.36	0.55
4:4:3:GLN:NE2	13:M:135:ARG:O	2.40	0.55
4:4:110:SER:OG	4:4:149:ASN:ND2	2.40	0.55
12:L:59:GLN:NE2	36:r:98:GLU:OE2	2.40	0.55
31:m:78:GLU:OE1	31:m:82:ARG:NH1	2.39	0.55
38:t:100:GLU:OE1	38:t:121:ARG:NH1	2.39	0.55
3:3:515:ARG:NH2	3:3:531:CYS:O	2.39	0.55
17:j:48:VAL:HG12	17:j:52:MET:HE2	1.89	0.54
39:u:10:ARG:HD2	39:u:15:PRO:HA	1.88	0.54
12:L:427:ILE:HG23	12:L:431:LEU:HD12	1.88	0.54
29:k:94:TYR:OH	29:k:151:HIS:ND1	2.37	0.54
1:1:243:ALA:HA	1:1:251:SER:HB3	1.89	0.54
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.89	0.54
49:L:1002:PC1:H372	51:W:201:CDL:H512	1.88	0.54
2:2:74:GLN:O	20:a:74:ARG:NH2	2.41	0.54
37:s:102:GLU:OE2	37:s:105:ARG:NH2	2.41	0.54
9:H:24:GLU:OE2	9:H:274:ARG:NH1	2.41	0.54
14:N:175:LEU:HD11	14:N:230:LEU:HB2	1.88	0.54
16:W:8:LEU:HD21	17:X:88:GLU:HB2	1.90	0.54
12:L:538:PRO:HB3	50:L:1001:3PE:H232	1.90	0.54
34:p:74:ASN:OD1	34:p:78:ASN:ND2	2.40	0.54
40:v:54:SER:HA	40:v:84:TYR:HB3	1.89	0.54
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.90	0.54
15:V:39:SER:OG	15:V:54:ARG:NH2	2.41	0.54
33:o:45:ASP:OD2	33:o:51:ARG:NH2	2.40	0.54
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.41	0.53
18:Y:100:ARG:NH1	18:Y:103:GLN:OE1	2.40	0.53
3:3:364:LEU:HD12	3:3:491:ASN:HB3	1.89	0.53
7:9:108:ARG:NH1	22:c:70:MET:O	2.39	0.53
8:A:73:LEU:HD13	10:J:55:MET:HE1	1.90	0.53
12:L:601:LEU:O	15:V:1:AYA:N	2.41	0.53
49:L:1002:PC1:H3A1	36:r:80:ILE:HG23	1.90	0.53
17:X:23:ASP:HB3	32:n:41:ARG:HH12	1.72	0.53
42:x:1:LYS:NZ	42:x:6:GLU:OE1	2.41	0.53
12:L:103:PHE:HB2	12:L:341:MET:HE3	1.90	0.53
14:N:128:LEU:HD13	14:N:216:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:11:ILE:HG22	17:X:77:VAL:HG22	1.90	0.53
7:9:64:GLU:OE1	7:9:136:ASN:ND2	2.41	0.53
22:c:28:GLU:O	22:c:32:THR:OG1	2.26	0.53
27:h:11:ARG:NH2	27:h:20:GLN:OE1	2.42	0.53
33:o:63:LEU:HD23	51:o:502:CDL:H112	1.89	0.53
37:s:8:TYR:OH	40:v:123:PRO:O	2.26	0.53
4:4:145:THR:OG1	4:4:181:TYR:OH	2.27	0.53
19:Z:5:ASP:HB3	19:Z:8:VAL:HG12	1.91	0.53
12:L:83:ASP:OD2	12:L:262:ARG:NH1	2.42	0.53
8:A:90:MET:HE1	10:J:155:ILE:HG13	1.91	0.52
15:V:54:ARG:HG2	15:V:57:ARG:HH22	1.72	0.52
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.91	0.52
3:3:585:VAL:O	22:c:61:THR:OG1	2.27	0.52
4:4:149:ASN:HD22	4:4:370:PRO:HB2	1.72	0.52
50:M:501:3PE:H271	50:M:501:3PE:H381	1.89	0.52
18:Y:29:HIS:HB3	18:Y:119:PRO:HD2	1.90	0.52
23:d:91:VAL:HG23	23:d:126:VAL:HG11	1.90	0.52
3:3:488:LYS:HD2	3:3:642:PHE:HE2	1.74	0.52
3:3:13:VAL:HG22	3:3:79:ILE:HD12	1.90	0.52
23:d:76:ARG:NH2	23:d:103:ASN:O	2.36	0.52
13:M:64:PRO:HB3	13:M:454:ILE:HG22	1.90	0.52
18:Y:71:ARG:NE	44:z:70:ASP:OD2	2.42	0.52
2:2:159:ASN:HB3	2:2:184:PRO:HB3	1.91	0.52
13:M:50:LEU:HA	16:W:86:ASN:HD21	1.75	0.52
13:M:457:PRO:O	41:w:84:ARG:NH1	2.43	0.52
12:L:373:LEU:HD22	12:L:431:LEU:HD11	1.91	0.52
4:4:200:HIS:NE2	7:9:124:GLU:OE1	2.43	0.52
14:N:249:LEU:HB3	14:N:254:LEU:HD12	1.91	0.52
4:4:233:ARG:NH2	7:9:23:GLN:O	2.40	0.52
12:L:203:MET:HB2	19:Z:113:GLN:HG3	1.91	0.52
50:L:1001:3PE:H221	40:v:88:ARG:HG2	1.91	0.52
52:X:101:ZMP:H19B	38:t:51:LYS:HG3	1.90	0.52
38:t:155:PRO:HG2	38:t:157:ARG:HE	1.73	0.52
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.92	0.51
33:o:52:PRO:HG2	33:o:56:ALA:HB2	1.92	0.51
33:o:66:THR:OG1	42:x:28:TRP:NE1	2.43	0.51
28:i:34:ARG:NH2	28:i:58:ARG:O	2.43	0.51
37:s:36:ARG:NH1	40:v:132:GLN:OE1	2.43	0.51
3:3:372:GLU:O	3:3:402:ASN:ND2	2.43	0.51
12:L:233:LEU:HD23	12:L:307:SER:HB3	1.93	0.51
52:X:101:ZMP:O6	38:t:12:GLN:NE2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:206:GLY:N	45:3:801:SF4:S2	2.79	0.51
14:N:159:ILE:HG21	14:N:278:LEU:HD11	1.93	0.51
51:V:203:CDL:OB4	51:V:204:CDL:OA7	2.29	0.51
16:W:143:ASN:HD22	30:l:29:PRO:HB3	1.75	0.51
17:j:37:MET:HE1	17:j:44:SER:HA	1.93	0.51
3:3:674:THR:O	3:3:679:ARG:NH1	2.43	0.51
4:4:391:ILE:O	4:4:430:ARG:NH1	2.44	0.51
12:L:184:LEU:HD13	13:M:393:ILE:HG21	1.93	0.51
51:L:1003:CDL:H621	13:M:372:SER:HB3	1.92	0.51
19:Z:64:HIS:NE2	41:w:92:GLU:OE1	2.38	0.51
23:d:176:ASP:OD1	23:d:180:ASN:ND2	2.44	0.51
3:3:187:ILE:HG13	3:3:189:LYS:HB2	1.92	0.51
4:4:101:PRO:O	4:4:105:ARG:NH1	2.43	0.51
4:4:305:ARG:NH1	35:q:21:LYS:O	2.44	0.51
7:9:7:LEU:HD23	27:h:112:LEU:HD11	1.92	0.51
19:Z:67:PHE:HD1	43:y:43:LEU:HD21	1.76	0.51
34:p:62:PRO:O	34:p:66:ARG:CB	2.59	0.51
1:1:120:GLU:OE2	1:1:236:ARG:NH1	2.43	0.51
4:4:106:LEU:HD13	4:4:391:ILE:HG21	1.91	0.51
12:L:543:THR:HG23	40:v:83:MET:HE1	1.92	0.51
19:Z:140:ASP:O	19:Z:161:ARG:NH1	2.43	0.51
40:v:62:TYR:HE2	40:v:72:ASN:HD21	1.58	0.51
12:L:375:ILE:HD12	12:L:458:LEU:HD11	1.93	0.50
6:6:63:ALA:HB2	6:6:69:MET:HE3	1.93	0.50
34:p:47:GLN:O	34:p:51:ASN:ND2	2.44	0.50
1:1:305:PRO:HG3	1:1:413:TRP:HB3	1.93	0.50
3:3:324:ASP:N	3:3:324:ASP:OD1	2.43	0.50
4:4:49:LEU:HD22	8:A:43:PRO:HB2	1.93	0.50
14:N:30:TRP:NE1	14:N:67:SER:OG	2.43	0.50
14:N:310:ASN:HB2	29:k:274:SER:HB3	1.93	0.50
3:3:324:ASP:HB3	3:3:571:ALA:HB1	1.93	0.50
4:4:184:VAL:O	7:9:60:ARG:NH1	2.44	0.50
9:H:316:PRO:HG3	35:q:56:ARG:HB3	1.93	0.50
12:L:90:VAL:HG22	12:L:129:LEU:HD22	1.93	0.50
13:M:9:MET:HE1	51:Y:201:CDL:H151	1.93	0.50
51:Y:201:CDL:H362	43:y:22:PHE:HZ	1.75	0.50
3:3:382:THR:HB	3:3:454:GLY:HA3	1.92	0.50
12:L:487:LYS:NZ	39:u:46:ALA:O	2.44	0.50
14:N:309:ASN:ND2	29:k:75:GLY:O	2.39	0.50
25:f:5:LYS:NZ	25:f:68:GLU:OE2	2.44	0.50
33:o:108:THR:OG1	33:o:111:GLU:OE1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:t:169:ILE:O	38:t:172:ARG:NH1	2.44	0.50
12:L:331:THR:HG22	12:L:335:PHE:HE1	1.76	0.50
29:k:135:LEU:HD21	29:k:149:VAL:HA	1.93	0.50
32:n:19:LYS:O	32:n:22:LYS:NZ	2.37	0.50
4:4:155:THR:HB	4:4:167:PHE:HA	1.94	0.50
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.44	0.50
49:L:1002:PC1:H341	51:W:201:CDL:H512	1.94	0.50
3:3:276:ARG:NH1	3:3:680:ALA:O	2.45	0.50
16:W:118:GLY:O	16:W:124:GLN:NE2	2.42	0.50
37:s:110:ARG:NH1	39:u:69:ASP:OD2	2.44	0.50
12:L:487:LYS:HE3	39:u:49:GLY:HA2	1.93	0.50
1:1:139:ARG:NE	1:1:141:GLU:OE1	2.43	0.49
3:3:379:LEU:HD13	3:3:384:PRO:HG3	1.93	0.49
6:6:44:SER:O	9:H:54:LYS:NZ	2.40	0.49
7:9:132:VAL:HG21	7:9:165:ILE:HG21	1.94	0.49
19:Z:3:SER:OG	19:Z:4:TRP:N	2.43	0.49
36:r:120:LYS:HB3	37:s:39:VAL:HG13	1.93	0.49
38:t:107:HIS:NE2	41:w:43:ASP:OD1	2.36	0.49
38:t:153:LEU:HD11	38:t:165:LEU:HD12	1.92	0.49
14:N:178:ILE:HG23	14:N:292:PHE:HE2	1.76	0.49
36:r:85:LEU:HD22	36:r:96:ILE:HD11	1.95	0.49
3:3:449:PRO:O	3:3:487:TRP:NE1	2.36	0.49
4:4:35:ASP:O	14:N:49:ASN:ND2	2.46	0.49
4:4:146:ARG:NH2	4:4:368:GLU:O	2.36	0.49
14:N:140:SER:HA	30:l:1:PRO:HD2	1.94	0.49
33:o:34:ILE:HG22	33:o:68:PHE:HB3	1.94	0.49
38:t:29:ARG:HD2	38:t:75:HIS:HD2	1.77	0.49
22:c:69:LEU:HD11	28:i:126:PRO:HG2	1.94	0.49
36:r:18:ARG:NH1	38:t:170:VAL:O	2.41	0.49
5:5:82:ASP:OD2	5:5:89:ARG:NH2	2.41	0.49
6:6:35:ASP:HB3	50:6:203:3PE:H331	1.95	0.49
3:3:101:HIS:HD2	4:4:342:MET:HE2	1.77	0.49
25:f:34:LEU:HD12	25:f:37:ILE:HD12	1.94	0.49
4:4:175:GLU:OE1	6:6:61:HIS:ND1	2.46	0.49
8:A:80:GLN:NE2	9:H:315:PRO:O	2.41	0.49
10:J:167:VAL:HG22	14:N:42:PRO:HG2	1.95	0.49
13:M:36:LEU:HB2	41:w:69:VAL:HG22	1.93	0.49
12:L:453:SER:HA	12:L:456:ARG:HH21	1.78	0.49
15:V:35:VAL:HG22	51:V:203:CDL:H342	1.95	0.49
23:d:10:LYS:NZ	26:g:126:ASP:OD2	2.40	0.49
12:L:69:LEU:HD13	13:M:451:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:s:21:MET:HE2	37:s:104:GLU:HG3	1.93	0.49
39:u:61:ASP:HB3	39:u:66:ILE:HB	1.94	0.49
3:3:99:ALA:O	3:3:134:LYS:NZ	2.43	0.48
3:3:119:GLN:HB2	3:3:123:PHE:HD2	1.78	0.48
13:M:151:PHE:HB2	50:M:501:3PE:H351	1.95	0.48
13:M:180:GLN:HA	13:M:248:LEU:HD21	1.95	0.48
29:k:25:ILE:HG12	29:k:168:VAL:HB	1.93	0.48
13:M:36:LEU:HD23	41:w:69:VAL:HA	1.96	0.48
49:M:503:PC1:H251	51:W:201:CDL:H381	1.94	0.48
51:V:203:CDL:H752	51:V:204:CDL:H191	1.94	0.48
27:h:13:TRP:O	35:q:27:ARG:NH2	2.45	0.48
3:3:319:ALA:HB3	3:3:345:THR:HG22	1.95	0.48
10:J:40:GLY:HA2	10:J:43:ILE:HD12	1.95	0.48
13:M:54:LEU:HD23	16:W:93:ILE:HG23	1.94	0.48
14:N:44:MET:HE2	14:N:130:LEU:HD12	1.94	0.48
18:Y:48:GLU:OE1	31:m:57:ARG:NH2	2.43	0.48
26:g:62:VAL:HG22	52:g:201:ZMP:H1A	1.95	0.48
38:t:137:LYS:HA	38:t:140:GLN:HG2	1.95	0.48
12:L:166:THR:OG1	40:v:87:ASN:ND2	2.42	0.48
8:A:70:ALA:HA	8:A:73:LEU:HD12	1.95	0.48
26:g:40:ARG:NH1	17:j:56:ASP:OD1	2.44	0.48
2:2:97:LYS:O	2:2:157:ASN:ND2	2.45	0.48
5:5:56:GLY:HA2	5:5:59:PRO:HD2	1.96	0.48
11:K:23:ARG:HG2	50:K:101:3PE:H11	1.94	0.48
12:L:172:ILE:HG21	13:M:408:LEU:HD12	1.95	0.48
50:M:502:3PE:H392	51:V:204:CDL:H861	1.95	0.48
51:M:505:CDL:H673	51:Y:201:CDL:H852	1.96	0.48
24:e:57:CYS:SG	24:e:58:SER:N	2.85	0.48
41:w:92:GLU:OE2	41:w:95:ARG:NH2	2.39	0.48
40:v:71:LEU:HD21	40:v:77:MET:HG2	1.95	0.48
1:1:144:ASN:O	1:1:148:ASN:HB2	2.13	0.48
3:3:41:CYS:O	3:3:161:ARG:NH2	2.34	0.48
49:9:401:PC1:H252	9:H:296:LEU:HD13	1.95	0.48
12:L:589:LEU:HD11	50:V:201:3PE:H232	1.95	0.48
17:X:23:ASP:HB2	32:n:43:PRO:HA	1.95	0.48
4:4:190:HIS:HD2	6:6:150:PRO:HD3	1.79	0.48
9:H:45:LEU:HD21	44:z:7:PRO:HB2	1.95	0.48
14:N:200:MET:HG3	14:N:269:GLU:HG3	1.96	0.48
51:W:201:CDL:H151	36:r:79:TRP:HB3	1.95	0.48
35:q:104:LYS:HB2	35:q:107:GLU:HB2	1.94	0.48
49:A:201:PC1:H291	10:J:152:TRP:HZ3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:4:LEU:HD13	15:V:7:GLN:HE21	1.79	0.48
30:l:105:PRO:HD3	35:q:81:ARG:HD3	1.94	0.48
35:q:92:GLU:HA	35:q:95:THR:HG22	1.95	0.48
13:M:70:MET:HG2	13:M:103:GLN:HE21	1.79	0.47
1:l:318:ASP:OD1	1:l:318:ASP:N	2.46	0.47
12:L:477:ILE:HD11	37:s:54:GLN:HA	1.95	0.47
51:L:1003:CDL:H473	51:W:201:CDL:H741	1.96	0.47
13:M:135:ARG:NH2	51:M:505:CDL:OB9	2.44	0.47
13:M:42:LEU:HD13	41:w:80:LEU:HD11	1.96	0.47
23:d:26:ALA:HA	23:d:31:GLY:HA3	1.96	0.47
6:6:43:SER:HB2	9:H:40:VAL:HG22	1.97	0.47
13:M:119:TYR:HE1	13:M:157:SER:HB2	1.80	0.47
14:N:338:PRO:HG3	51:Y:201:CDL:H792	1.97	0.47
12:L:25:ASN:HD22	12:L:29:PHE:HE2	1.62	0.47
1:l:378:ARG:NE	3:3:132:GLU:OE2	2.33	0.47
3:3:193:SER:H	3:3:196:SER:HB3	1.79	0.47
3:3:296:TRP:HE1	3:3:592:LEU:HB3	1.79	0.47
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.34	0.47
13:M:337:VAL:HG11	13:M:345:ALA:HB2	1.97	0.47
29:k:30:ASN:O	29:k:126:ARG:NH2	2.43	0.47
31:m:42:LEU:HD11	31:m:46:ARG:HH21	1.78	0.47
2:2:111:ARG:HD3	2:2:151:ALA:HB3	1.96	0.47
7:9:162:GLU:HB3	28:i:109:ILE:HG12	1.97	0.47
15:V:49:LEU:HA	15:V:52:VAL:HG22	1.97	0.47
28:i:78:ASP:HB3	28:i:81:MET:HG3	1.95	0.47
2:2:34:ILE:HD11	20:a:52:LEU:HD22	1.97	0.47
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.95	0.47
13:M:281:ASP:HB3	13:M:284:SER:HB2	1.97	0.47
14:N:20:VAL:HG11	14:N:137:ALA:HB1	1.96	0.47
26:g:21:SER:OG	26:g:30:ARG:NH1	2.48	0.47
3:3:371:VAL:HG22	3:3:450:MET:HE1	1.96	0.47
43:y:8:ARG:HG3	43:y:10:HIS:H	1.79	0.47
14:N:110:PRO:HD3	14:N:160:LEU:HD23	1.96	0.46
6:6:155:ALA:HB2	7:9:137:PHE:HD2	1.79	0.46
24:e:23:CYS:SG	24:e:25:ARG:N	2.86	0.46
29:k:108:TYR:OH	29:k:164:LEU:O	2.31	0.46
41:w:36:ASN:HB3	41:w:39:GLU:HG3	1.97	0.46
18:Y:6:LEU:HD12	35:q:90:LEU:HD22	1.96	0.46
1:l:365:CYS:HB3	45:l:500:SF4:S3	2.56	0.46
15:V:124:VAL:HG22	50:V:202:3PE:H362	1.97	0.46
29:k:165:PRO:O	29:k:248:TRP:NE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:104:ARG:NH1	35:q:84:GLN:OE1	2.48	0.46
22:c:42:ARG:HD3	22:c:49:VAL:HG12	1.98	0.46
12:L:570:GLN:OE1	14:N:167:TRP:NE1	2.48	0.46
49:L:1002:PC1:H32	49:M:503:PC1:H142	1.96	0.46
18:Y:171:MET:SD	51:Y:201:CDL:OB4	2.74	0.46
23:d:26:ALA:HB3	23:d:47:VAL:HG13	1.97	0.46
23:d:201:VAL:HG22	23:d:237:LEU:HD23	1.97	0.46
17:j:62:ILE:HG12	17:j:79:TYR:HE2	1.81	0.46
29:k:308:TYR:HD1	29:k:317:ILE:HG23	1.81	0.46
6:6:59:MET:HE2	6:6:69:MET:HE1	1.98	0.46
8:A:69:ILE:HD11	9:H:144:VAL:HG13	1.98	0.46
11:K:46:LEU:O	11:K:50:ASN:HB2	2.15	0.46
13:M:1:FME:HG2	13:M:111:THR:HG21	1.98	0.46
12:L:129:LEU:HA	12:L:132:VAL:HG22	1.97	0.46
13:M:279:GLN:HB2	13:M:285:LEU:HD12	1.98	0.46
15:V:1:AYA:HM2	15:V:3:THR:HG22	1.98	0.46
33:o:60:ARG:HE	51:o:502:CDL:HA31	1.80	0.46
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.45	0.46
11:K:73:LEU:HD11	14:N:41:ILE:HG13	1.98	0.46
51:V:203:CDL:H322	51:V:203:CDL:H532	1.98	0.46
2:2:102:VAL:HG22	2:2:154:VAL:HG12	1.98	0.46
3:3:148:THR:HG23	3:3:150:MET:HE3	1.98	0.46
8:A:3:LEU:HD13	9:H:96:ILE:HG21	1.98	0.46
12:L:66:TRP:NE1	49:M:503:PC1:O12	2.37	0.46
12:L:542:LEU:HB2	40:v:83:MET:HE3	1.97	0.46
1:1:91:LYS:HG2	1:1:219:PRO:HB2	1.97	0.45
13:M:369:LEU:HD12	13:M:370:PRO:HD2	1.98	0.45
18:Y:144:ARG:NE	30:l:58:GLU:OE2	2.49	0.45
5:5:119:SER:OG	5:5:131:GLU:OE2	2.25	0.45
12:L:396:ILE:HG21	12:L:490:ALA:HB2	1.98	0.45
12:L:558:LEU:HD13	12:L:561:ILE:HD11	1.98	0.45
1:1:154:ARG:HA	20:a:58:LEU:HD21	1.98	0.45
1:1:361:GLN:O	1:1:366:ARG:NH1	2.49	0.45
12:L:73:THR:HB	12:L:194:ASN:HD21	1.80	0.45
12:L:173:LEU:HD12	13:M:405:LEU:HD21	1.99	0.45
3:3:174:THR:HG22	3:3:183:VAL:HG22	1.98	0.45
28:i:54:GLN:HB3	28:i:58:ARG:HB2	1.99	0.45
43:y:46:ARG:NH2	43:y:52:GLU:OE2	2.48	0.45
3:3:283:MET:HB2	3:3:560:ILE:HB	1.98	0.45
3:3:320:GLY:O	3:3:498:SER:OG	2.34	0.45
3:3:426:PRO:HB2	3:3:656:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:347:ILE:HG12	12:L:354:GLN:HG2	1.99	0.45
3:3:259:ASN:O	3:3:262:TRP:N	2.44	0.45
4:4:61:VAL:HG11	6:6:96:MET:HE1	1.99	0.45
8:A:74:PRO:HG2	10:J:147:TYR:HE2	1.81	0.45
12:L:397:GLU:HB3	12:L:482:MET:HE1	1.97	0.45
51:L:1003:CDL:H181	13:M:442:LEU:HD13	1.98	0.45
13:M:321:LEU:HD11	49:M:503:PC1:H3E1	1.97	0.45
17:X:54:MET:HG3	17:X:76:ILE:HD13	1.98	0.45
40:v:47:TYR:OH	40:v:77:MET:O	2.27	0.45
4:4:84:HIS:NE2	6:6:130:TYR:OH	2.39	0.45
4:4:111:MET:HE2	4:4:181:TYR:HE2	1.82	0.45
4:4:208:MET:HE1	35:q:10:PRO:HD3	1.98	0.45
4:4:387:TYR:CZ	5:5:164:LYS:HE3	2.52	0.45
5:5:39:GLN:HB2	5:5:51:CYS:HB2	1.99	0.45
51:L:1003:CDL:H631	13:M:445:LEU:HD22	1.97	0.45
29:k:48:LEU:HD22	29:k:121:GLY:HA3	1.99	0.45
3:3:569:LYS:HG3	3:3:571:ALA:HB2	1.97	0.45
10:J:163:ILE:HG21	14:N:12:THR:HG21	1.98	0.45
12:L:362:LEU:N	12:L:431:LEU:O	2.50	0.45
12:L:536:LEU:HG	12:L:540:MET:HE2	1.99	0.45
14:N:206:ILE:HD12	14:N:346:LEU:HD11	1.98	0.45
16:W:114:MET:HE2	16:W:121:PRO:HD2	1.98	0.45
19:Z:52:GLU:HA	19:Z:55:HIS:HD2	1.82	0.45
17:j:65:ILE:H	17:j:65:ILE:HG13	1.67	0.45
12:L:604:PHE:O	14:N:150:ASN:ND2	2.50	0.45
14:N:347:GLU:HB2	33:o:82:MET:HE2	1.99	0.45
29:k:32:CYS:HB2	29:k:179:VAL:HG13	1.99	0.45
3:3:478:ARG:HH21	3:3:485:GLY:HA2	1.82	0.44
5:5:72:PHE:O	5:5:124:TYR:OH	2.33	0.44
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.98	0.44
4:4:154:VAL:HG11	4:4:225:LEU:HD21	1.98	0.44
18:Y:3:ILE:HD11	35:q:104:LYS:HE3	1.99	0.44
24:e:17:GLU:HG2	24:e:67:ARG:HB3	1.98	0.44
3:3:332:LYS:NZ	3:3:505:LEU:O	2.40	0.44
4:4:94:LYS:HD2	4:4:102:TYR:HE2	1.81	0.44
12:L:13:ILE:HD11	51:W:201:CDL:H622	2.00	0.44
23:d:153:GLU:HG3	23:d:165:ILE:HD13	1.99	0.44
2:2:10:ARG:HH21	21:b:77:LYS:HG2	1.82	0.44
2:2:50:VAL:HG12	2:2:69:VAL:HG22	2.00	0.44
3:3:632:ARG:NH1	24:e:59:ASP:H	2.13	0.44
4:4:224:GLU:OE2	7:9:40:TYR:OH	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:19:ASP:HB2	21:b:22:ASP:HB2	2.00	0.44
28:i:9:ARG:HA	28:i:12:GLN:HG2	2.00	0.44
9:H:42:PRO:HD2	9:H:46:LEU:HD23	1.98	0.44
18:Y:17:VAL:HG12	18:Y:19:VAL:HG22	2.00	0.44
52:g:201:ZMP:O7	17:j:44:SER:OG	2.30	0.44
10:J:45:LEU:HD23	10:J:50:SER:HA	2.00	0.44
11:K:96:LEU:HD23	14:N:51:ARG:HH11	1.81	0.44
16:W:133:ILE:HD13	30:l:37:LYS:HG2	1.99	0.44
52:X:101:ZMP:H7	38:t:46:ARG:HB3	2.00	0.44
27:h:5:ARG:HA	27:h:8:GLN:HB3	1.98	0.44
7:9:97:GLU:OE2	28:i:131:ARG:NH2	2.47	0.44
12:L:10:VAL:HG21	36:r:78:VAL:HG22	1.98	0.44
12:L:123:LEU:HB2	12:L:150:MET:HE2	2.00	0.44
13:M:181:TYR:O	19:Z:152:ARG:NH1	2.51	0.44
14:N:289:ASN:HA	14:N:292:PHE:CE1	2.53	0.44
3:3:329:ILE:HD12	3:3:329:ILE:HA	1.83	0.44
4:4:203:LEU:HD22	4:4:207:LEU:HD23	1.99	0.44
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.99	0.44
6:6:109:GLU:HG2	6:6:111:ARG:HD3	1.99	0.44
7:9:99:ARG:HH12	21:b:40:ALA:HB3	1.83	0.44
29:k:30:ASN:N	29:k:33:SER:OG	2.44	0.44
35:q:88:GLU:OE1	35:q:127:ARG:NH2	2.51	0.44
2:2:99:HIS:CE1	2:2:101:GLN:HE21	2.36	0.44
2:2:121:GLN:HE21	2:2:128:VAL:HG23	1.82	0.44
9:H:162:LEU:HD21	9:H:237:PHE:HE1	1.80	0.44
51:L:1003:CDL:H512	51:L:1003:CDL:H541	1.81	0.44
15:V:12:PRO:HB2	15:V:15:THR:HG21	1.98	0.44
18:Y:125:SER:HA	31:m:53:PRO:HG3	2.00	0.44
22:c:33:ARG:NH1	22:c:77:ASP:OD1	2.51	0.44
23:d:133:SER:OG	23:d:134:HIS:N	2.50	0.44
3:3:518:PRO:HB2	3:3:538:PRO:HD3	1.99	0.43
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.36	0.43
14:N:222:ASN:HD21	14:N:240:MET:HB3	1.82	0.43
4:4:13:GLN:HB3	4:4:19:MET:HE1	2.01	0.43
13:M:18:SER:HB2	13:M:23:ILE:HG22	2.00	0.43
13:M:232:ALA:O	13:M:237:LYS:NZ	2.51	0.43
51:V:203:CDL:H202	51:V:203:CDL:H372	1.99	0.43
19:Z:159:LYS:NZ	33:o:112:VAL:O	2.49	0.43
39:u:18:THR:HG22	39:u:20:SER:H	1.83	0.43
41:w:114:ASP:HB3	41:w:117:LYS:HG2	2.00	0.43
2:2:40:GLU:HB2	20:a:67:SER:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:362:TYR:OH	3:3:504:ASP:OD1	2.31	0.43
50:6:203:3PE:H2I3	9:H:49:ILE:HG13	2.01	0.43
9:H:55:LEU:HD13	9:H:221:ALA:HB2	2.01	0.43
14:N:119:THR:HG22	14:N:176:ARG:HB3	2.00	0.43
17:X:13:ASP:O	17:X:17:TYR:HB2	2.18	0.43
18:Y:39:ASN:HB3	35:q:72:PRO:HG2	2.00	0.43
3:3:215:PHE:HB2	7:9:98:PRO:HD3	1.99	0.43
3:3:284:VAL:HG12	3:3:559:VAL:HG22	2.01	0.43
4:4:343:GLU:O	4:4:347:HIS:ND1	2.36	0.43
7:9:132:VAL:HG11	7:9:169:ILE:HD11	2.00	0.43
10:J:152:TRP:HZ2	14:N:19:ILE:HG12	1.83	0.43
18:Y:82:THR:HA	18:Y:85:TRP:CD1	2.53	0.43
19:Z:141:ARG:HG3	41:w:112:CYS:HB2	2.01	0.43
22:c:42:ARG:NH1	22:c:46:GLN:O	2.51	0.43
23:d:167:LYS:HB2	23:d:229:ALA:HA	1.99	0.43
30:l:74:ARG:NH2	35:q:93:GLU:OE2	2.51	0.43
12:L:161:ARG:HA	38:t:91:GLU:HG3	2.01	0.43
13:M:9:MET:HB3	51:Y:201:CDL:H261	2.01	0.43
13:M:78:MET:HE2	41:w:61:VAL:HG22	1.99	0.43
13:M:122:PHE:HZ	13:M:206:LYS:HG3	1.83	0.43
14:N:128:LEU:HD11	14:N:213:SER:HA	2.00	0.43
51:V:203:CDL:H221	51:V:203:CDL:H192	1.74	0.43
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.83	0.43
7:9:155:LEU:HB3	21:b:36:ASN:HD22	1.83	0.43
17:j:17:TYR:HA	17:j:20:LYS:HG2	2.01	0.43
29:k:30:ASN:H	29:k:33:SER:HG	1.62	0.43
34:p:70:ALA:HB2	40:v:10:PRO:HG2	2.01	0.43
40:v:30:ARG:O	40:v:34:TYR:N	2.48	0.43
2:2:116:ILE:HG23	2:2:169:ILE:HG21	1.99	0.43
12:L:434:GLN:NE2	32:n:51:ARG:O	2.51	0.43
15:V:139:LYS:HG3	15:V:140:VAL:HG13	1.99	0.43
1:1:361:GLN:N	45:1:500:SF4:S4	2.89	0.43
7:9:78:ILE:H	7:9:78:ILE:HG13	1.63	0.43
13:M:60:SER:HB2	13:M:457:PRO:HA	2.00	0.43
15:V:11:ILE:HB	15:V:20:LYS:HD3	2.00	0.43
15:V:124:VAL:HA	50:V:202:3PE:H351	2.01	0.43
22:c:32:THR:HB	26:g:127:PRO:HG2	2.01	0.43
23:d:166:ILE:HG22	23:d:168:PRO:HD3	2.00	0.43
1:1:425:GLU:OE2	1:1:429:ARG:NH2	2.48	0.43
3:3:525:LEU:HD21	3:3:600:ILE:HD11	2.01	0.43
3:3:555:PRO:HG3	28:i:137:TRP:HZ2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:60:ILE:HG21	10:J:168:ILE:HG21	2.00	0.43
9:H:73:LEU:HD22	50:H:401:3PE:H3I3	2.01	0.43
12:L:419:THR:HA	12:L:422:TYR:CE1	2.53	0.43
14:N:4:ILE:HD11	29:k:9:ILE:HG23	2.00	0.43
24:e:68:TYR:HB2	24:e:72:GLN:HB2	2.00	0.43
33:o:6:GLN:HE22	33:o:85:VAL:HG11	1.84	0.43
3:3:157:THR:O	3:3:161:ARG:NE	2.40	0.43
7:9:151:LYS:HE2	7:9:155:LEU:HD11	2.00	0.43
8:A:3:LEU:HD22	50:H:401:3PE:H32	2.01	0.43
12:L:236:ALA:HB1	12:L:248:HIS:CE1	2.54	0.43
15:V:3:THR:HA	15:V:6:HIS:HB2	2.01	0.43
5:5:211:GLN:OE1	22:c:54:LYS:NZ	2.41	0.42
10:J:54:LEU:HD23	10:J:54:LEU:HA	1.89	0.42
12:L:542:LEU:HB3	13:M:278:ARG:HD3	1.99	0.42
21:b:31:ARG:HD3	28:i:123:GLN:HE21	1.84	0.42
29:k:104:ARG:NH1	29:k:126:ARG:O	2.51	0.42
3:3:163:ALA:HA	3:3:167:ALA:HB3	2.00	0.42
3:3:175:THR:HG21	3:3:186:TYR:HB2	2.00	0.42
5:5:211:GLN:NE2	25:f:115:ILE:O	2.42	0.42
12:L:563:PRO:HA	50:M:501:3PE:H392	2.00	0.42
13:M:116:ILE:HD12	13:M:116:ILE:HA	1.92	0.42
13:M:155:ALA:HB1	49:M:504:PC1:H2H1	2.00	0.42
14:N:275:SER:HB3	15:V:136:ALA:HB3	2.00	0.42
51:W:201:CDL:H171	19:Z:47:VAL:HG21	2.02	0.42
2:2:24:THR:OG1	2:2:27:ASN:OD1	2.37	0.42
13:M:403:THR:HA	13:M:406:TYR:CE1	2.54	0.42
16:W:138:LYS:HA	30:l:27:ARG:HB3	2.01	0.42
29:k:309:ASN:N	29:k:314:ASP:OD2	2.50	0.42
3:3:425:SER:HA	3:3:426:PRO:HD3	1.94	0.42
4:4:51:PHE:HZ	4:4:411:LEU:HD21	1.84	0.42
4:4:155:THR:HG21	4:4:170:MET:HB2	2.01	0.42
5:5:182:ARG:HD2	26:g:100:THR:HA	2.00	0.42
7:9:1:THR:N	27:h:104:GLU:O	2.36	0.42
7:9:164:GLU:HG3	28:i:88:ARG:HG3	2.02	0.42
49:A:201:PC1:H132	49:A:201:PC1:H111	1.89	0.42
10:J:128:TYR:O	30:l:31:ARG:NH2	2.52	0.42
12:L:316:THR:HA	12:L:319:ILE:HG12	2.00	0.42
30:l:6:GLN:NE2	30:l:14:ASP:OD1	2.44	0.42
3:3:365:ASN:N	3:3:491:ASN:OD1	2.52	0.42
4:4:292:ASP:OD1	4:4:292:ASP:N	2.50	0.42
5:5:88:ASN:HA	5:5:112:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:L:1003:CDL:H401	51:L:1003:CDL:H671	2.01	0.42
51:L:1003:CDL:H642	51:L:1003:CDL:H562	2.02	0.42
13:M:225:ILE:HD13	13:M:331:ASN:HB2	2.00	0.42
13:M:290:SER:HA	13:M:319:HIS:HE2	1.83	0.42
19:Z:84:MET:HE1	19:Z:152:ARG:HD2	2.02	0.42
35:q:55:GLU:OE1	35:q:58:ARG:NH2	2.51	0.42
3:3:46:LEU:HD11	3:3:202:ILE:HD12	2.01	0.42
3:3:272:ASP:OD2	3:3:683:THR:OG1	2.29	0.42
9:H:171:GLN:HG3	35:q:52:TRP:HB2	2.02	0.42
18:Y:21:SER:N	44:z:51:ASP:OD1	2.52	0.42
4:4:323:ILE:HD12	4:4:324:LYS:HG3	2.01	0.42
7:9:53:GLU:OE2	28:i:34:ARG:NH2	2.42	0.42
9:H:70:MET:HE1	10:J:27:ILE:HG22	2.01	0.42
9:H:100:LEU:HD23	9:H:160:PHE:HB2	2.02	0.42
12:L:171:ALA:HA	12:L:232:TRP:HB2	2.02	0.42
12:L:253:VAL:HB	12:L:310:LEU:HD11	2.02	0.42
13:M:346:ARG:NE	40:v:68:ASP:OD2	2.48	0.42
51:M:505:CDL:H791	51:M:505:CDL:H571	2.02	0.42
4:4:50:ASN:N	8:A:43:PRO:O	2.46	0.42
11:K:47:MET:HE3	11:K:47:MET:HB2	1.83	0.42
43:y:14:VAL:HA	43:y:17:PRO:HD2	2.01	0.42
13:M:328:CYS:HB3	13:M:437:MET:HE1	2.02	0.42
13:M:426:ILE:HB	38:t:101:TRP:HH2	1.85	0.42
19:Z:10:PRO:O	36:r:94:TYR:OH	2.31	0.42
28:i:44:TYR:OH	28:i:113:HIS:N	2.45	0.42
29:k:27:VAL:HG22	29:k:170:ILE:HB	2.02	0.42
3:3:115:ASP:O	3:3:119:GLN:HG2	2.20	0.41
3:3:140:LYS:HD3	3:3:150:MET:HG3	2.02	0.41
3:3:394:ARG:HD3	3:3:394:ARG:HA	1.85	0.41
4:4:104:ASP:HB3	4:4:190:HIS:ND1	2.34	0.41
7:9:74:GLU:HB2	21:b:44:ILE:HD13	2.02	0.41
12:L:316:THR:HG23	12:L:325:ALA:HB2	2.02	0.41
13:M:165:ILE:HG21	14:N:268:GLN:HA	2.02	0.41
13:M:332:SER:O	13:M:336:ARG:NH1	2.53	0.41
15:V:76:SER:HA	15:V:79:VAL:HG22	2.02	0.41
18:Y:165:ARG:HH12	33:o:90:MET:HE1	1.84	0.41
23:d:100:GLU:HB2	23:d:105:ASP:HA	2.01	0.41
24:e:96:SER:OG	24:e:97:LYS:N	2.53	0.41
3:3:579:ARG:HB2	3:3:636:VAL:HG22	2.02	0.41
4:4:285:VAL:H	7:9:2:TYR:HA	1.85	0.41
13:M:447:LEU:HD11	49:M:503:PC1:H3F1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:499:GLN:HE21	3:3:503:LEU:HD11	1.84	0.41
4:4:71:GLU:HB3	4:4:410:MET:HG2	2.02	0.41
6:6:58:GLU:HG2	6:6:151:PRO:O	2.20	0.41
11:K:55:LEU:HA	11:K:55:LEU:HD23	1.87	0.41
51:W:201:CDL:H372	51:W:201:CDL:H841	2.03	0.41
18:Y:33:ALA:HB2	18:Y:119:PRO:HG3	2.02	0.41
51:Y:201:CDL:H512	51:Y:201:CDL:H542	1.90	0.41
29:k:213:GLU:O	29:k:217:LYS:NZ	2.52	0.41
30:l:7:LYS:NZ	33:o:8:ARG:O	2.52	0.41
32:n:23:ILE:HG22	32:n:49:ALA:HB2	2.01	0.41
1:1:258:ILE:HG22	1:1:262:VAL:HG21	2.03	0.41
5:5:31:GLU:OE2	25:f:46:TYR:OH	2.32	0.41
12:L:1:FME:HB2	12:L:1:FME:HE2	1.78	0.41
13:M:216:LEU:HD23	13:M:287:ALA:HB1	2.03	0.41
13:M:243:MET:HB3	13:M:301:ILE:HG21	2.02	0.41
21:b:49:VAL:HG22	21:b:90:GLN:HG3	2.03	0.41
23:d:153:GLU:HG3	23:d:165:ILE:HG21	2.02	0.41
40:v:137:ASN:O	40:v:142:ARG:NH1	2.52	0.41
4:4:204:PRO:HG2	4:4:207:LEU:HB2	2.03	0.41
5:5:137:MET:HA	5:5:161:PRO:HD2	2.02	0.41
11:K:20:LEU:HB3	12:L:592:LEU:HB2	2.02	0.41
13:M:301:ILE:HA	13:M:309:TYR:HE1	1.85	0.41
15:V:32:GLY:HA3	15:V:59:THR:HA	2.03	0.41
1:1:66:ARG:HA	1:1:74:PRO:HA	2.02	0.41
11:K:38:LEU:O	11:K:42:ILE:HG12	2.20	0.41
13:M:158:LEU:HD23	14:N:283:ALA:HB1	2.01	0.41
16:W:119:ASP:HB3	30:l:50:ARG:HD2	2.01	0.41
29:k:57:HIS:HB3	29:k:60:ASP:HB2	2.02	0.41
36:r:17:LEU:HD11	38:t:162:LEU:HD22	2.02	0.41
4:4:103:PHE:HA	4:4:106:LEU:HD12	2.03	0.41
12:L:589:LEU:HD12	15:V:41:ALA:HA	2.02	0.41
49:L:1002:PC1:H372	49:L:1002:PC1:H341	1.85	0.41
30:l:14:ASP:OD1	30:l:14:ASP:N	2.54	0.41
33:o:5:ARG:NH2	33:o:89:ASP:OD1	2.54	0.41
3:3:399:TRP:HA	3:3:404:LEU:HB3	2.02	0.41
3:3:622:ARG:NH2	24:e:73:GLU:OE2	2.54	0.41
5:5:137:MET:HE3	5:5:152:LEU:HB2	2.03	0.41
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.55	0.41
12:L:97:THR:HG21	12:L:125:LEU:HD22	2.02	0.41
12:L:290:MET:O	12:L:523:SER:OG	2.30	0.41
51:L:1003:CDL:H461	49:M:503:PC1:H252	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:V:203:CDL:H731	51:V:204:CDL:H171	2.03	0.41
16:W:138:LYS:HB2	16:W:143:ASN:HD21	1.85	0.41
18:Y:144:ARG:NH2	30:l:54:GLU:O	2.54	0.41
34:p:14:PRO:HG2	34:p:17:LEU:HD12	2.03	0.41
1:1:96:ASN:ND2	1:1:187:GLY:O	2.51	0.41
3:3:347:GLU:OE2	3:3:455:SER:OG	2.32	0.41
7:9:27:TRP:HB3	7:9:30:LEU:HD12	2.02	0.41
8:A:71:LEU:O	10:J:147:TYR:OH	2.31	0.41
50:H:401:3PE:H322	10:J:54:LEU:HD21	2.02	0.41
10:J:153:LEU:HD21	11:K:62:ILE:HG13	2.03	0.41
12:L:88:MET:HB2	12:L:326:PHE:HE2	1.86	0.41
13:M:204:MET:O	13:M:209:LEU:N	2.48	0.41
13:M:278:ARG:NH2	40:v:83:MET:SD	2.94	0.41
13:M:326:LEU:HD23	13:M:326:LEU:HA	1.93	0.41
17:X:63:PRO:O	17:X:67:ALA:N	2.53	0.41
28:i:44:TYR:HH	28:i:113:HIS:H	1.66	0.41
50:i:201:3PE:H2E2	50:i:201:3PE:H3D2	2.02	0.41
29:k:56:ILE:HD11	29:k:78:SER:HA	2.03	0.41
29:k:93:SER:HB3	29:k:138:MET:HE3	2.03	0.41
33:o:42:GLY:HA3	33:o:61:GLN:HG2	2.03	0.41
40:v:96:VAL:HB	40:v:101:MET:HE3	2.01	0.41
41:w:77:VAL:HA	41:w:80:LEU:HG	2.01	0.41
41:w:80:LEU:HA	41:w:81:PRO:HD3	1.94	0.41
3:3:80:LEU:HB3	3:3:83:SER:HB3	2.02	0.41
3:3:503:LEU:HD21	3:3:509:PRO:HB3	2.03	0.41
50:6:203:3PE:H3A2	50:6:203:3PE:H3D2	1.87	0.41
7:9:175:TYR:CZ	27:h:38:PRO:HG3	2.56	0.41
50:A:202:3PE:H381	9:H:295:PRO:HB3	2.02	0.41
10:J:103:MET:HE3	10:J:115:ILE:HG13	2.03	0.41
12:L:375:ILE:HG12	39:u:32:MET:SD	2.61	0.41
14:N:210:ILE:HG22	14:N:333:SER:HB3	2.03	0.41
14:N:284:ILE:HD13	14:N:284:ILE:HA	1.93	0.41
27:h:51:ASN:OD1	27:h:56:ARG:NE	2.51	0.41
30:l:6:GLN:OE1	30:l:15:HIS:NE2	2.53	0.41
2:2:149:VAL:O	2:2:190:ARG:NH2	2.45	0.40
3:3:522:LEU:HD22	3:3:537:LEU:HD11	2.03	0.40
4:4:66:MET:HE1	4:4:414:VAL:HG11	2.02	0.40
8:A:84:LEU:HD11	31:m:45:ASN:HD22	1.86	0.40
28:i:60:ARG:HH22	28:i:95:ASP:HA	1.86	0.40
3:3:105:CYS:SG	3:3:117:GLN:NE2	2.87	0.40
4:4:151:ILE:O	4:4:155:THR:OG1	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:78:LEU:HB3	5:5:130:TYR:HB3	2.03	0.40
5:5:109:THR:OG1	5:5:110:TYR:N	2.54	0.40
49:9:401:PC1:H351	9:H:187:ILE:HD12	2.02	0.40
9:H:31:MET:HE1	9:H:272:TRP:HB2	2.03	0.40
9:H:311:LEU:O	35:q:54:ARG:NH2	2.54	0.40
12:L:316:THR:HB	12:L:395:ILE:HG23	2.03	0.40
13:M:147:LEU:HG	14:N:298:TYR:HE2	1.86	0.40
13:M:305:THR:O	13:M:308:SER:OG	2.38	0.40
17:X:20:LYS:HD2	32:n:18:TYR:CZ	2.56	0.40
52:X:101:ZMP:H17	52:X:101:ZMP:H15	1.60	0.40
29:k:314:ASP:HB2	29:k:317:ILE:HD11	2.04	0.40
1:1:298:ILE:HB	1:1:335:ILE:HB	2.04	0.40
4:4:296:ARG:HH21	4:4:420:THR:HG21	1.85	0.40
5:5:116:PRO:HB3	5:5:141:PHE:HD2	1.87	0.40
14:N:93:MET:HE3	14:N:97:LEU:HG	2.04	0.40
18:Y:90:TYR:HA	44:z:34:ARG:HG2	2.03	0.40
29:k:172:VAL:HG12	29:k:174:VAL:HG23	2.04	0.40
3:3:146:VAL:HG22	3:3:200:ILE:HD11	2.03	0.40
3:3:194:GLU:HG3	3:3:389:PRO:HB3	2.02	0.40
4:4:424:VAL:O	4:4:427:GLU:HG2	2.21	0.40
5:5:175:ARG:NH2	5:5:186:GLU:OE2	2.37	0.40
9:H:87:ILE:HG22	9:H:95:LEU:HD23	2.03	0.40
13:M:405:LEU:HD23	13:M:405:LEU:HA	1.94	0.40
19:Z:166:ARG:NH2	41:w:121:PRO:O	2.37	0.40
1:1:20:ARG:HH12	2:2:201:SER:HB2	1.86	0.40
1:1:79:TRP:CD1	1:1:221:THR:HG21	2.56	0.40
4:4:149:ASN:ND2	4:4:370:PRO:HB2	2.35	0.40
6:6:84:ASP:OD1	9:H:58:LYS:NZ	2.42	0.40
10:J:169:MET:HE2	10:J:169:MET:HB3	1.94	0.40
13:M:75:LEU:HD23	13:M:440:HIS:CE1	2.56	0.40
14:N:115:VAL:HG12	14:N:180:ALA:HB1	2.02	0.40
29:k:133:VAL:HG12	29:k:205:VAL:HG12	2.03	0.40
35:q:30:SER:OG	35:q:31:GLY:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	428/464 (92%)	407 (95%)	21 (5%)	0	100	100
2	2	211/246 (86%)	190 (90%)	21 (10%)	0	100	100
3	3	686/727 (94%)	659 (96%)	27 (4%)	0	100	100
4	4	414/463 (89%)	399 (96%)	15 (4%)	0	100	100
5	5	206/266 (77%)	194 (94%)	12 (6%)	0	100	100
6	6	154/223 (69%)	145 (94%)	9 (6%)	0	100	100
7	9	174/217 (80%)	165 (95%)	9 (5%)	0	100	100
8	A	106/115 (92%)	98 (92%)	8 (8%)	0	100	100
9	H	309/318 (97%)	295 (96%)	14 (4%)	0	100	100
10	J	163/175 (93%)	158 (97%)	5 (3%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	567 (94%)	37 (6%)	0	100	100
13	M	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
14	N	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
15	V	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
16	W	137/189 (72%)	133 (97%)	4 (3%)	0	100	100
17	X	85/157 (54%)	83 (98%)	2 (2%)	0	100	100
17	j	80/157 (51%)	76 (95%)	4 (5%)	0	100	100
18	Y	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
19	Z	169/175 (97%)	163 (96%)	6 (4%)	0	100	100
20	a	42/109 (38%)	42 (100%)	0	0	100	100
21	b	93/124 (75%)	90 (97%)	3 (3%)	0	100	100
22	c	124/170 (73%)	117 (94%)	7 (6%)	0	100	100
23	d	289/380 (76%)	279 (96%)	10 (4%)	0	100	100
24	e	84/99 (85%)	82 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	f	111/116 (96%)	106 (96%)	5 (4%)	0	100	100
26	g	112/140 (80%)	107 (96%)	5 (4%)	0	100	100
27	h	92/114 (81%)	87 (95%)	5 (5%)	0	100	100
28	i	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
29	k	317/355 (89%)	298 (94%)	19 (6%)	0	100	100
30	l	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
31	m	78/84 (93%)	72 (92%)	6 (8%)	0	100	100
32	n	77/98 (79%)	71 (92%)	6 (8%)	0	100	100
33	o	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
34	p	126/130 (97%)	120 (95%)	6 (5%)	0	100	100
35	q	137/144 (95%)	133 (97%)	4 (3%)	0	100	100
36	r	95/128 (74%)	88 (93%)	7 (7%)	0	100	100
37	s	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
38	t	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
39	u	63/108 (58%)	62 (98%)	1 (2%)	0	100	100
40	v	153/186 (82%)	143 (94%)	10 (6%)	0	100	100
41	w	99/154 (64%)	91 (92%)	8 (8%)	0	100	100
42	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
43	y	48/58 (83%)	46 (96%)	2 (4%)	0	100	100
44	z	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	8045/9247 (87%)	7683 (96%)	362 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	344/368 (94%)	344 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	183/210 (87%)	183 (100%)	0	100	100
3	3	578/608 (95%)	578 (100%)	0	100	100
4	4	363/391 (93%)	362 (100%)	1 (0%)	86	83
5	5	189/230 (82%)	188 (100%)	1 (0%)	81	80
6	6	132/181 (73%)	131 (99%)	1 (1%)	73	77
7	9	151/179 (84%)	150 (99%)	1 (1%)	76	78
8	A	99/103 (96%)	99 (100%)	0	100	100
9	H	273/278 (98%)	273 (100%)	0	100	100
10	J	136/144 (94%)	136 (100%)	0	100	100
11	K	86/86 (100%)	86 (100%)	0	100	100
12	L	538/538 (100%)	538 (100%)	0	100	100
13	M	411/411 (100%)	411 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	V	101/102 (99%)	101 (100%)	0	100	100
16	W	122/160 (76%)	122 (100%)	0	100	100
17	X	80/141 (57%)	80 (100%)	0	100	100
17	j	76/141 (54%)	76 (100%)	0	100	100
18	Y	154/155 (99%)	154 (100%)	0	100	100
19	Z	155/157 (99%)	155 (100%)	0	100	100
20	a	43/93 (46%)	43 (100%)	0	100	100
21	b	79/97 (81%)	79 (100%)	0	100	100
22	c	113/150 (75%)	113 (100%)	0	100	100
23	d	255/326 (78%)	255 (100%)	0	100	100
24	e	76/82 (93%)	76 (100%)	0	100	100
25	f	101/102 (99%)	101 (100%)	0	100	100
26	g	107/124 (86%)	107 (100%)	0	100	100
27	h	84/96 (88%)	84 (100%)	0	100	100
28	i	131/131 (100%)	131 (100%)	0	100	100
29	k	283/309 (92%)	282 (100%)	1 (0%)	84	81
30	l	94/95 (99%)	94 (100%)	0	100	100
31	m	69/72 (96%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	n	61/76 (80%)	61 (100%)	0	100	100
33	o	107/109 (98%)	107 (100%)	0	100	100
34	p	114/116 (98%)	114 (100%)	0	100	100
35	q	119/122 (98%)	119 (100%)	0	100	100
36	r	95/122 (78%)	94 (99%)	1 (1%)	65	74
37	s	110/120 (92%)	110 (100%)	0	100	100
38	t	159/161 (99%)	159 (100%)	0	100	100
39	u	59/84 (70%)	59 (100%)	0	100	100
40	v	140/160 (88%)	140 (100%)	0	100	100
41	w	92/130 (71%)	92 (100%)	0	100	100
42	x	44/67 (66%)	44 (100%)	0	100	100
43	y	46/54 (85%)	46 (100%)	0	100	100
44	z	59/59 (100%)	59 (100%)	0	100	100
All	All	7126/7955 (90%)	7120 (100%)	6 (0%)	87	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	323	ILE
5	5	92	ILE
6	6	54	CYS
7	9	78	ILE
29	k	96	LEU
36	r	75	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
1	1	150	GLN
1	1	437	HIS
2	2	101	GLN
2	2	155	GLN
3	3	255	HIS
3	3	401	HIS
3	3	475	GLN

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Mol	Chain	Res	Type
3	3	621	ASN
3	3	665	GLN
4	4	135	GLN
4	4	149	ASN
4	4	217	ASN
4	4	252	ASN
5	5	19	HIS
5	5	144	ASN
5	5	160	HIS
6	6	82	GLN
6	6	94	ASN
9	H	247	HIS
9	H	317	GLN
11	K	25	HIS
12	L	135	ASN
12	L	199	GLN
12	L	210	ASN
12	L	248	HIS
12	L	270	ASN
12	L	354	GLN
12	L	434	GLN
12	L	446	ASN
12	L	479	GLN
12	L	506	ASN
13	M	138	ASN
13	M	169	ASN
13	M	333	ASN
13	M	374	ASN
13	M	390	ASN
13	M	415	GLN
13	M	422	HIS
14	N	172	GLN
14	N	289	ASN
15	V	7	GLN
16	W	143	ASN
18	Y	29	HIS
18	Y	76	HIS
19	Z	55	HIS
19	Z	106	GLN
20	a	40	ASN
21	b	36	ASN
21	b	51	GLN

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Mol	Chain	Res	Type
22	c	43	ASN
23	d	44	GLN
23	d	87	HIS
23	d	103	ASN
23	d	184	ASN
24	e	47	ASN
26	g	69	ASN
29	k	141	GLN
29	k	200	GLN
29	k	204	ASN
29	k	251	GLN
30	l	97	HIS
33	o	12	GLN
34	p	47	GLN
40	v	55	GLN
40	v	66	HIS
40	v	87	ASN
40	v	126	GLN
40	v	155	HIS
41	w	45	HIS
41	w	57	ASN
41	w	103	HIS
42	x	9	HIS
42	x	46	ASN
43	y	10	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	AYA	h	1	27	6,7,8	1.38	1 (16%)	6,8,10	1.54	1 (16%)
4	2MR	4	85	4	10,12,13	2.40	3 (30%)	5,13,15	1.35	0
13	FME	M	1	13	8,9,10	1.04	1 (12%)	8,9,11	0.92	0
11	FME	K	1	11	8,9,10	0.94	0	8,9,11	1.26	1 (12%)
15	AYA	V	1	15	6,7,8	1.26	1 (16%)	6,8,10	1.62	2 (33%)
12	FME	L	1	12	8,9,10	0.98	0	8,9,11	1.00	0
29	SEP	k	36	29	8,9,10	1.63	1 (12%)	7,12,14	1.19	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	AYA	h	1	27	-	1/5/6/8	-
4	2MR	4	85	4	-	0/10/13/15	-
13	FME	M	1	13	-	3/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
15	AYA	V	1	15	-	2/5/6/8	-
12	FME	L	1	12	-	3/7/9/11	-
29	SEP	k	36	29	-	4/6/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	4.96	1.43	1.33
4	4	85	2MR	CZ-NE	4.70	1.44	1.34
29	k	36	SEP	P-O1P	3.55	1.61	1.50
27	h	1	AYA	CA-N	-2.88	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.28	1.41	1.46
15	V	1	AYA	CA-N	-2.22	1.44	1.46
13	M	1	FME	CA-N	-2.18	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	h	1	AYA	CB-CA-N	3.67	113.82	109.68
15	V	1	AYA	CA-N-CT	2.58	124.83	121.50
11	K	1	FME	C-CA-N	2.38	114.09	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	k	36	SEP	OG-CB-CA	2.30	110.39	108.14
15	V	1	AYA	CB-CA-N	2.25	112.22	109.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
12	L	1	FME	N-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
27	h	1	AYA	O-C-CA-CB
29	k	36	SEP	CB-OG-P-O1P
29	k	36	SEP	CB-OG-P-O2P
29	k	36	SEP	CB-OG-P-O3P
11	K	1	FME	CA-CB-CG-SD
15	V	1	AYA	OT-CT-N-CA
15	V	1	AYA	CM-CT-N-CA
11	K	1	FME	N-CA-CB-CG
13	M	1	FME	N-CA-CB-CG
12	L	1	FME	CA-CB-CG-SD
12	L	1	FME	C-CA-CB-CG
13	M	1	FME	CB-CA-N-CN
11	K	1	FME	C-CA-CB-CG
29	k	36	SEP	CA-CB-OG-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0
15	V	1	AYA	2	0
12	L	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 2 are monoatomic - leaving 42 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
50	3PE	N	401	-	50,50,50	0.32	0	53,55,55	0.54	1 (1%)
50	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.30	0
50	3PE	A	202	-	50,50,50	0.30	0	53,55,55	0.35	0
52	ZMP	X	101	17	25,30,36	0.80	1 (4%)	29,37,45	1.11	1 (3%)
45	SF4	3	802	3	0,12,12	-	-	-	-	-
49	PC1	A	201	-	36,36,53	0.37	0	42,44,61	0.63	1 (2%)
49	PC1	6	202	-	45,45,53	0.32	0	51,53,61	0.32	0
45	SF4	3	801	3	0,12,12	-	-	-	-	-
50	3PE	M	501	-	39,39,50	0.33	0	42,44,55	0.35	0
50	3PE	M	502	-	43,43,50	0.32	0	46,48,55	0.29	0
51	CDL	V	204	-	84,84,99	0.29	0	90,96,111	0.26	0
45	SF4	9	403	7	0,12,12	-	-	-	-	-
51	CDL	M	505	-	89,89,99	0.31	0	95,101,111	0.38	1 (1%)
45	SF4	9	402	7	0,12,12	-	-	-	-	-
51	CDL	V	203	-	93,93,99	0.30	0	99,105,111	0.31	0
50	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.38	0
51	CDL	L	1003	-	99,99,99	0.26	0	105,111,111	0.29	0
50	3PE	6	203	-	50,50,50	0.31	0	53,55,55	0.29	0
47	FES	3	803	3	0,4,4	-	-	-	-	-
50	3PE	L	1004	-	30,30,50	0.41	0	33,35,55	0.81	2 (6%)
51	CDL	Y	201	-	99,99,99	0.27	0	105,111,111	0.33	0
54	NDP	d	401	-	51,52,52	0.39	0	71,80,80	0.40	0
50	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.44	0
50	3PE	H	401	-	50,50,50	0.30	0	53,55,55	0.43	0
45	SF4	6	201	6	0,12,12	-	-	-	-	-
50	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.36	0
51	CDL	z	101	-	57,57,99	0.33	0	63,69,111	0.34	0
46	FMN	1	501	-	33,33,33	1.19	3 (9%)	48,50,50	1.32	8 (16%)
50	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.35	0
52	ZMP	g	201	-	28,33,36	0.70	2 (7%)	32,40,45	1.25	4 (12%)
47	FES	2	300	2	0,4,4	-	-	-	-	-
49	PC1	M	503	-	53,53,53	0.29	0	59,61,61	0.35	0
50	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.35	0
51	CDL	W	201	-	99,99,99	0.26	0	105,111,111	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	MYR	s	201	37	13,14,15	0.17	0	12,13,15	0.16	0
49	PC1	L	1002	-	53,53,53	0.30	0	59,61,61	0.63	2 (3%)
49	PC1	9	401	-	53,53,53	0.30	0	59,61,61	0.54	2 (3%)
55	AMP	k	501	-	25,25,25	1.42	4 (16%)	37,38,38	2.05	8 (21%)
51	CDL	o	502	-	74,74,99	0.30	0	80,86,111	0.44	1 (1%)
49	PC1	M	504	-	53,53,53	0.30	0	59,61,61	0.45	0
45	SF4	1	500	1	0,12,12	-	-	-		
50	3PE	p	201	-	26,26,50	0.49	0	29,31,55	0.55	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	3PE	N	401	-	-	12/54/54/54	-
50	3PE	i	201	-	-	3/54/54/54	-
50	3PE	A	202	-	-	9/54/54/54	-
52	ZMP	X	101	17	-	18/35/37/43	-
45	SF4	3	802	3	-	-	0/6/5/5
49	PC1	A	201	-	-	6/40/40/57	-
49	PC1	6	202	-	-	14/49/49/57	-
45	SF4	3	801	3	-	-	0/6/5/5
50	3PE	M	501	-	-	14/43/43/54	-
50	3PE	M	502	-	-	10/47/47/54	-
51	CDL	V	204	-	1/1/9/9	33/95/95/110	-
45	SF4	9	403	7	-	-	0/6/5/5
51	CDL	M	505	-	-	26/100/100/110	-
45	SF4	9	402	7	-	-	0/6/5/5
51	CDL	V	203	-	-	37/104/104/110	-
50	3PE	o	501	-	-	4/34/34/54	-
51	CDL	L	1003	-	1/1/9/9	30/110/110/110	-
50	3PE	L	1004	-	-	10/34/34/54	-
50	3PE	6	203	-	-	15/54/54/54	-
47	FES	3	803	3	-	-	0/1/1/1
51	CDL	Y	201	-	1/1/9/9	26/110/110/110	-
54	NDP	d	401	-	-	2/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	3PE	K	101	-	-	9/43/43/54	-
50	3PE	H	401	-	-	16/54/54/54	-
50	3PE	L	1001	-	-	10/54/54/54	-
51	CDL	z	101	-	-	16/68/68/110	-
45	SF4	6	201	6	-	-	0/6/5/5
46	FMN	1	501	-	-	9/18/18/18	0/3/3/3
50	3PE	V	202	-	-	9/40/40/54	-
52	ZMP	g	201	-	-	7/38/40/43	-
47	FES	2	300	2	-	-	0/1/1/1
49	PC1	M	503	-	-	13/57/57/57	-
50	3PE	V	201	-	-	9/38/38/54	-
51	CDL	W	201	-	-	28/110/110/110	-
56	MYR	s	201	37	-	4/12/12/13	-
49	PC1	L	1002	-	-	24/57/57/57	-
49	PC1	9	401	-	-	18/57/57/57	-
55	AMP	k	501	-	-	7/10/26/26	0/3/3/3
51	CDL	o	502	-	2/2/9/9	21/85/85/110	-
49	PC1	M	504	-	-	20/57/57/57	-
45	SF4	1	500	1	-	-	0/6/5/5
50	3PE	p	201	-	-	8/27/27/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	k	501	AMP	C5-C4	4.87	1.47	1.39
55	k	501	AMP	C5-C6	2.75	1.48	1.41
46	1	501	FMN	C4A-N5	2.67	1.36	1.30
52	X	101	ZMP	C9-C10	2.35	1.53	1.50
55	k	501	AMP	C5-N7	-2.32	1.34	1.39
55	k	501	AMP	C8-N7	2.12	1.35	1.31
46	1	501	FMN	C10-N1	2.11	1.37	1.33
52	g	201	ZMP	C9-C10	2.05	1.52	1.50
52	g	201	ZMP	C10-S1	-2.02	1.71	1.76
46	1	501	FMN	C4A-C10	-2.02	1.38	1.44

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	k	501	AMP	C5-C4-N3	-6.80	117.35	126.72
55	k	501	AMP	N3-C4-N9	5.67	136.81	127.17
55	k	501	AMP	C2-N3-C4	4.17	122.03	111.83
46	1	501	FMN	C4-N3-C2	-3.64	119.18	125.64
52	X	101	ZMP	O1-C10-C9	-3.37	120.09	123.98
55	k	501	AMP	N3-C2-N1	-3.34	123.53	128.58
55	k	501	AMP	C4-C5-N7	-3.08	107.06	110.58
46	1	501	FMN	C4'-C3'-C2'	-3.05	108.49	113.57
46	1	501	FMN	O4-C4-C4A	-2.97	118.68	126.53
52	g	201	ZMP	C15-C14-C13	-2.93	107.51	112.39
52	g	201	ZMP	O1-C10-C9	-2.93	120.60	123.98
52	g	201	ZMP	C14-C15-N2	-2.73	106.19	112.00
46	1	501	FMN	C4A-C10-N10	2.72	120.38	116.48
46	1	501	FMN	C4A-C4-N3	2.61	119.90	113.25
49	L	1002	PC1	C2-O21-C21	2.60	124.02	117.80
49	L	1002	PC1	O21-C2-C1	2.58	117.59	108.34
50	L	1004	3PE	C2-O21-C21	2.37	123.46	117.80
46	1	501	FMN	C4-C4A-C10	2.34	120.95	116.93
55	k	501	AMP	C5-N7-C8	2.33	107.12	103.45
55	k	501	AMP	C4-N9-C8	2.31	108.16	105.74
49	A	201	PC1	C2-O21-C21	2.30	123.30	117.80
51	o	502	CDL	CB4-OB6-CB5	2.25	123.19	117.80
46	1	501	FMN	C4A-C10-N1	-2.24	119.10	124.59
50	N	401	3PE	C2-O21-C21	2.24	123.15	117.80
55	k	501	AMP	C1'-N9-C8	-2.22	122.17	127.09
52	g	201	ZMP	C9-C10-S1	2.18	116.00	113.40
50	p	201	3PE	O12-P-O14	2.12	119.08	110.83
46	1	501	FMN	C5A-C9A-N10	2.08	119.85	117.97
50	L	1004	3PE	O21-C2-C3	2.08	115.80	108.34
51	M	505	CDL	CB4-OB6-CB5	2.07	122.74	117.80
49	9	401	PC1	C2-O21-C21	2.03	122.66	117.80
49	9	401	PC1	O21-C2-C1	2.02	115.58	108.34

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
51	L	1003	CDL	CB4
51	V	204	CDL	CB4
51	Y	201	CDL	CB4
51	o	502	CDL	CA4
51	o	502	CDL	CB4

All (497) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	501	FMN	N10-C1'-C2'-O2'
46	1	501	FMN	N10-C1'-C2'-C3'
46	1	501	FMN	C1'-C2'-C3'-C4'
46	1	501	FMN	C5'-O5'-P-O2P
46	1	501	FMN	C5'-O5'-P-O3P
49	6	202	PC1	C11-O13-P-O12
49	6	202	PC1	C11-O13-P-O14
49	6	202	PC1	C11-O13-P-O11
49	6	202	PC1	C1-O11-P-O14
49	9	401	PC1	C1-O11-P-O12
49	9	401	PC1	C1-O11-P-O14
49	9	401	PC1	C1-O11-P-O13
49	A	201	PC1	C11-O13-P-O14
49	A	201	PC1	C11-O13-P-O11
49	L	1002	PC1	C11-O13-P-O14
49	L	1002	PC1	C1-O11-P-O12
49	L	1002	PC1	O13-C11-C12-N
49	L	1002	PC1	C2-C1-O11-P
49	M	503	PC1	C11-O13-P-O12
49	M	503	PC1	C11-O13-P-O11
49	M	504	PC1	C11-O13-P-O12
49	M	504	PC1	C11-O13-P-O14
49	M	504	PC1	C11-O13-P-O11
49	M	504	PC1	C1-O11-P-O12
50	6	203	3PE	C1-O11-P-O12
50	6	203	3PE	C1-O11-P-O13
50	6	203	3PE	C1-O11-P-O14
50	6	203	3PE	O13-C11-C12-N
50	A	202	3PE	C1-O11-P-O14
50	H	401	3PE	C1-O11-P-O13
50	H	401	3PE	C11-O13-P-O11
50	H	401	3PE	C11-O13-P-O12
50	H	401	3PE	C11-O13-P-O14
50	H	401	3PE	O13-C11-C12-N
50	K	101	3PE	C1-O11-P-O12
50	K	101	3PE	C1-O11-P-O13
50	K	101	3PE	C1-O11-P-O14
50	L	1001	3PE	C11-O13-P-O11
50	L	1001	3PE	O13-C11-C12-N
50	L	1004	3PE	C1-O11-P-O13
50	L	1004	3PE	C11-O13-P-O11
50	L	1004	3PE	C11-O13-P-O12
50	L	1004	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
50	L	1004	3PE	C2-C1-O11-P
50	M	501	3PE	C1-O11-P-O12
50	M	501	3PE	O13-C11-C12-N
50	M	502	3PE	C1-O11-P-O14
50	N	401	3PE	C11-O13-P-O12
50	V	201	3PE	C11-O13-P-O11
50	V	201	3PE	C11-O13-P-O14
50	V	201	3PE	O13-C11-C12-N
50	V	202	3PE	C11-O13-P-O11
50	V	202	3PE	O13-C11-C12-N
50	i	201	3PE	C11-O13-P-O11
50	i	201	3PE	C11-O13-P-O12
50	o	501	3PE	C11-O13-P-O11
50	o	501	3PE	C11-O13-P-O14
50	p	201	3PE	C1-O11-P-O12
50	p	201	3PE	C1-O11-P-O13
50	p	201	3PE	C1-O11-P-O14
51	L	1003	CDL	C1-CA2-OA2-PA1
51	L	1003	CDL	CA3-OA5-PA1-OA2
51	L	1003	CDL	CA3-OA5-PA1-OA3
51	L	1003	CDL	CA3-OA5-PA1-OA4
51	M	505	CDL	CA2-OA2-PA1-OA5
51	M	505	CDL	CA3-OA5-PA1-OA3
51	M	505	CDL	CB2-OB2-PB2-OB3
51	M	505	CDL	CB2-OB2-PB2-OB5
51	M	505	CDL	CB3-OB5-PB2-OB3
51	V	203	CDL	CA2-OA2-PA1-OA4
51	V	203	CDL	CB2-OB2-PB2-OB3
51	V	203	CDL	CB2-OB2-PB2-OB4
51	V	203	CDL	CB2-OB2-PB2-OB5
51	V	203	CDL	CB3-OB5-PB2-OB4
51	V	203	CDL	OB6-CB4-CB6-OB8
51	V	204	CDL	CA2-OA2-PA1-OA3
51	V	204	CDL	CA2-OA2-PA1-OA4
51	V	204	CDL	CA2-OA2-PA1-OA5
51	V	204	CDL	CB2-OB2-PB2-OB3
51	V	204	CDL	CB2-OB2-PB2-OB4
51	V	204	CDL	CB2-OB2-PB2-OB5
51	V	204	CDL	CB3-OB5-PB2-OB2
51	V	204	CDL	CB3-OB5-PB2-OB3
51	W	201	CDL	CA2-OA2-PA1-OA5
51	W	201	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
51	W	201	CDL	CB2-OB2-PB2-OB5
51	W	201	CDL	CB3-OB5-PB2-OB2
51	W	201	CDL	CB3-OB5-PB2-OB3
51	W	201	CDL	OB5-CB3-CB4-OB6
51	Y	201	CDL	CA2-OA2-PA1-OA3
51	Y	201	CDL	CA2-OA2-PA1-OA4
51	Y	201	CDL	CA2-OA2-PA1-OA5
51	Y	201	CDL	CB2-OB2-PB2-OB3
51	Y	201	CDL	CB3-OB5-PB2-OB2
51	Y	201	CDL	CB3-OB5-PB2-OB3
51	o	502	CDL	CA2-OA2-PA1-OA3
51	o	502	CDL	CA2-OA2-PA1-OA5
51	o	502	CDL	CA3-OA5-PA1-OA4
51	o	502	CDL	CB2-OB2-PB2-OB3
51	o	502	CDL	CB2-OB2-PB2-OB4
51	o	502	CDL	CB2-OB2-PB2-OB5
51	z	101	CDL	CA2-OA2-PA1-OA4
51	z	101	CDL	CA2-OA2-PA1-OA5
51	z	101	CDL	CA3-OA5-PA1-OA3
51	z	101	CDL	CB2-OB2-PB2-OB3
51	z	101	CDL	CB2-OB2-PB2-OB4
51	z	101	CDL	CB2-OB2-PB2-OB5
52	X	101	ZMP	O4-C17-C18-C21
52	X	101	ZMP	C16-C17-C18-C21
52	X	101	ZMP	O4-C17-C18-C19
52	X	101	ZMP	C16-C17-C18-C19
52	X	101	ZMP	C16-C17-C18-C20
52	X	101	ZMP	O3-C16-C17-O4
52	X	101	ZMP	C17-C16-N2-C15
52	X	101	ZMP	S1-C11-C12-N1
52	g	201	ZMP	S1-C11-C12-N1
52	g	201	ZMP	C12-C11-S1-C10
52	g	201	ZMP	O1-C10-S1-C11
52	g	201	ZMP	C9-C10-S1-C11
52	g	201	ZMP	C7-C8-C9-C10
55	k	501	AMP	C5'-O5'-P-O1P
55	k	501	AMP	C5'-O5'-P-O2P
55	k	501	AMP	C5'-O5'-P-O3P
56	s	201	MYR	O1-C1-C2-C3
56	s	201	MYR	C1-C2-C3-C4
52	X	101	ZMP	O3-C16-N2-C15
55	k	501	AMP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
50	M	502	3PE	C2-C1-O11-P
51	V	203	CDL	CA2-C1-CB2-OB2
51	W	201	CDL	CA2-C1-CB2-OB2
49	M	504	PC1	C11-C12-N-C14
49	A	201	PC1	C22-C23-C24-C25
51	W	201	CDL	O1-C1-CB2-OB2
51	V	204	CDL	OA6-CA4-CA6-OA8
50	N	401	3PE	C21-C22-C23-C24
55	k	501	AMP	O4'-C4'-C5'-O5'
49	6	202	PC1	C11-C12-N-C14
49	M	504	PC1	C11-C12-N-C15
51	o	502	CDL	CB7-C71-C72-C73
51	V	203	CDL	O1-C1-CB2-OB2
50	N	401	3PE	C31-C32-C33-C34
51	L	1003	CDL	CB5-C51-C52-C53
51	V	203	CDL	CB5-C51-C52-C53
51	Y	201	CDL	C82-C83-C84-C85
51	M	505	CDL	CB5-C51-C52-C53
51	L	1003	CDL	O1-C1-CB2-OB2
49	L	1002	PC1	C2A-C2B-C2C-C2D
50	6	203	3PE	C37-C38-C39-C3A
49	6	202	PC1	C11-C12-N-C15
50	A	202	3PE	C2C-C2D-C2E-C2F
51	M	505	CDL	C58-C59-C60-C61
49	M	504	PC1	C3A-C3B-C3C-C3D
50	i	201	3PE	C29-C2A-C2B-C2C
51	Y	201	CDL	C15-C16-C17-C18
51	L	1003	CDL	C56-C57-C58-C59
51	M	505	CDL	C78-C79-C80-C81
51	W	201	CDL	C35-C36-C37-C38
49	L	1002	PC1	C33-C34-C35-C36
51	M	505	CDL	C71-C72-C73-C74
50	M	501	3PE	C27-C28-C29-C2A
51	L	1003	CDL	C22-C23-C24-C25
50	6	203	3PE	C3A-C3B-C3C-C3D
50	K	101	3PE	C34-C35-C36-C37
51	V	203	CDL	C43-C44-C45-C46
51	V	203	CDL	C52-C53-C54-C55
51	V	204	CDL	C34-C35-C36-C37
49	6	202	PC1	C3B-C3C-C3D-C3E
50	6	203	3PE	C3B-C3C-C3D-C3E
51	W	201	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
49	L	1002	PC1	C38-C39-C3A-C3B
50	6	203	3PE	C2D-C2E-C2F-C2G
51	V	203	CDL	C79-C80-C81-C82
51	W	201	CDL	C31-C32-C33-C34
52	X	101	ZMP	C6-C7-C8-C9
49	L	1002	PC1	C37-C38-C39-C3A
49	9	401	PC1	C2C-C2D-C2E-C2F
51	L	1003	CDL	C41-C42-C43-C44
49	6	202	PC1	C11-C12-N-C13
51	z	101	CDL	CA5-C11-C12-C13
51	Y	201	CDL	C63-C64-C65-C66
51	L	1003	CDL	C76-C77-C78-C79
51	W	201	CDL	C15-C16-C17-C18
51	V	203	CDL	C39-C40-C41-C42
51	Y	201	CDL	C59-C60-C61-C62
51	L	1003	CDL	C21-C22-C23-C24
49	M	504	PC1	C11-C12-N-C13
51	V	204	CDL	C52-C53-C54-C55
50	6	203	3PE	C35-C36-C37-C38
50	K	101	3PE	C36-C37-C38-C39
51	W	201	CDL	C72-C73-C74-C75
51	V	203	CDL	C32-C33-C34-C35
50	V	201	3PE	C21-C22-C23-C24
51	L	1003	CDL	CA2-C1-CB2-OB2
51	z	101	CDL	CA2-C1-CB2-OB2
51	V	204	CDL	C22-C23-C24-C25
50	M	502	3PE	O11-C1-C2-C3
51	W	201	CDL	OB5-CB3-CB4-CB6
50	p	201	3PE	C22-C23-C24-C25
51	W	201	CDL	C62-C63-C64-C65
51	V	203	CDL	CB3-CB4-CB6-OB8
51	V	204	CDL	CA3-CA4-CA6-OA8
51	Y	201	CDL	CA3-CA4-CA6-OA8
51	V	203	CDL	C19-C20-C21-C22
49	M	503	PC1	C27-C28-C29-C2A
51	Y	201	CDL	CB7-C71-C72-C73
49	9	401	PC1	C22-C21-O21-C2
50	V	202	3PE	C2-C1-O11-P
50	A	202	3PE	C38-C39-C3A-C3B
50	K	101	3PE	C24-C25-C26-C27
46	1	501	FMN	C5'-O5'-P-O1P
50	V	202	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
49	M	503	PC1	C26-C27-C28-C29
51	o	502	CDL	OB5-CB3-CB4-OB6
51	Y	201	CDL	C56-C57-C58-C59
50	V	202	3PE	C26-C27-C28-C29
51	Y	201	CDL	C14-C15-C16-C17
51	W	201	CDL	O1-C1-CA2-OA2
49	M	503	PC1	C3E-C3F-C3G-C3H
51	M	505	CDL	C84-C85-C86-C87
52	X	101	ZMP	O4-C17-C18-C20
51	Y	201	CDL	C11-C12-C13-C14
51	W	201	CDL	CA7-C31-C32-C33
49	M	504	PC1	C2-C1-O11-P
50	K	101	3PE	C2-C1-O11-P
51	z	101	CDL	CB4-CB3-OB5-PB2
51	V	204	CDL	C54-C55-C56-C57
51	L	1003	CDL	OB5-CB3-CB4-CB6
51	V	203	CDL	OA5-CA3-CA4-CA6
49	M	503	PC1	C24-C25-C26-C27
51	V	204	CDL	C71-C72-C73-C74
50	M	502	3PE	C21-C22-C23-C24
49	M	504	PC1	C36-C37-C38-C39
52	X	101	ZMP	N2-C16-C17-O4
51	L	1003	CDL	C80-C81-C82-C83
51	V	204	CDL	C15-C16-C17-C18
50	L	1001	3PE	O11-C1-C2-O21
51	o	502	CDL	C71-C72-C73-C74
51	z	101	CDL	O1-C1-CB2-OB2
52	X	101	ZMP	O1-C10-S1-C11
51	M	505	CDL	C77-C78-C79-C80
51	L	1003	CDL	C19-C20-C21-C22
49	L	1002	PC1	C36-C37-C38-C39
49	A	201	PC1	C21-C22-C23-C24
50	M	501	3PE	C31-C32-C33-C34
51	o	502	CDL	CA7-C31-C32-C33
50	M	501	3PE	C23-C24-C25-C26
51	L	1003	CDL	C34-C35-C36-C37
51	Y	201	CDL	C81-C82-C83-C84
52	X	101	ZMP	C9-C10-S1-C11
50	H	401	3PE	O11-C1-C2-C3
50	L	1001	3PE	C23-C24-C25-C26
50	A	202	3PE	C24-C25-C26-C27
50	H	401	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
49	9	401	PC1	O22-C21-O21-C2
49	9	401	PC1	C3E-C3F-C3G-C3H
52	X	101	ZMP	C5-C6-C7-C8
50	A	202	3PE	O11-C1-C2-O21
50	V	201	3PE	C1-C2-C3-O31
51	V	204	CDL	CB3-CB4-CB6-OB8
46	1	501	FMN	O2'-C2'-C3'-C4'
51	V	204	CDL	OB6-CB4-CB6-OB8
50	H	401	3PE	C26-C27-C28-C29
49	L	1002	PC1	C25-C26-C27-C28
51	V	203	CDL	C23-C24-C25-C26
50	o	501	3PE	C21-C22-C23-C24
50	L	1001	3PE	C3B-C3C-C3D-C3E
51	Y	201	CDL	C13-C14-C15-C16
54	d	401	NDP	O4D-C1D-N1N-C6N
49	L	1002	PC1	O11-C1-C2-C3
50	L	1001	3PE	O11-C1-C2-C3
50	L	1004	3PE	O11-C1-C2-C3
46	1	501	FMN	O2'-C2'-C3'-O3'
52	X	101	ZMP	C19-C18-C21-O5
51	z	101	CDL	C1-CB2-OB2-PB2
50	L	1004	3PE	C33-C34-C35-C36
49	L	1002	PC1	O11-C1-C2-O21
50	H	401	3PE	O11-C1-C2-O21
50	L	1004	3PE	O11-C1-C2-O21
51	L	1003	CDL	OB5-CB3-CB4-OB6
51	V	203	CDL	OA5-CA3-CA4-OA6
51	V	203	CDL	OB5-CB3-CB4-OB6
51	Y	201	CDL	OB5-CB3-CB4-OB6
51	V	203	CDL	C22-C23-C24-C25
50	V	201	3PE	O21-C2-C3-O31
51	Y	201	CDL	OA6-CA4-CA6-OA8
51	W	201	CDL	CA3-CA4-CA6-OA8
51	z	101	CDL	CA3-CA4-CA6-OA8
51	M	505	CDL	C81-C82-C83-C84
49	6	202	PC1	O31-C31-C32-C33
49	L	1002	PC1	C3A-C3B-C3C-C3D
49	6	202	PC1	C1-O11-P-O12
49	6	202	PC1	C1-O11-P-O13
49	L	1002	PC1	C11-O13-P-O12
49	L	1002	PC1	C11-O13-P-O11
49	L	1002	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
49	L	1002	PC1	C1-O11-P-O13
49	M	504	PC1	C1-O11-P-O14
49	M	504	PC1	C1-O11-P-O13
50	6	203	3PE	C11-O13-P-O14
50	A	202	3PE	C1-O11-P-O13
50	L	1001	3PE	C11-O13-P-O14
50	L	1004	3PE	C1-O11-P-O14
50	M	501	3PE	C1-O11-P-O13
50	M	501	3PE	C1-O11-P-O14
50	M	502	3PE	C1-O11-P-O12
50	M	502	3PE	C1-O11-P-O13
50	N	401	3PE	C11-O13-P-O11
50	N	401	3PE	C11-O13-P-O14
50	N	401	3PE	O13-C11-C12-N
50	V	202	3PE	C1-O11-P-O12
50	V	202	3PE	C1-O11-P-O13
50	V	202	3PE	C1-O11-P-O14
50	V	202	3PE	C11-O13-P-O14
51	L	1003	CDL	CA2-OA2-PA1-OA3
51	L	1003	CDL	CA2-OA2-PA1-OA4
51	L	1003	CDL	CA2-OA2-PA1-OA5
51	L	1003	CDL	CB2-OB2-PB2-OB3
51	M	505	CDL	CA2-OA2-PA1-OA3
51	M	505	CDL	CA2-OA2-PA1-OA4
51	M	505	CDL	CB2-OB2-PB2-OB4
51	V	203	CDL	CA2-OA2-PA1-OA3
51	V	203	CDL	CA2-OA2-PA1-OA5
51	V	203	CDL	CB3-OB5-PB2-OB2
51	V	203	CDL	CB3-OB5-PB2-OB3
51	V	204	CDL	CA3-OA5-PA1-OA3
51	V	204	CDL	CB3-OB5-PB2-OB4
51	W	201	CDL	CA2-OA2-PA1-OA3
51	W	201	CDL	CB3-OB5-PB2-OB4
51	o	502	CDL	CA2-OA2-PA1-OA4
51	o	502	CDL	CA3-OA5-PA1-OA2
51	o	502	CDL	CA3-OA5-PA1-OA3
51	o	502	CDL	CB3-OB5-PB2-OB3
51	V	204	CDL	C73-C74-C75-C76
49	9	401	PC1	C2-C1-O11-P
50	H	401	3PE	C2-C1-O11-P
51	L	1003	CDL	CA4-CA3-OA5-PA1
51	M	505	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
55	k	501	AMP	C4'-C5'-O5'-P
51	V	203	CDL	C71-C72-C73-C74
50	L	1001	3PE	C35-C36-C37-C38
49	L	1002	PC1	C3B-C3C-C3D-C3E
49	M	503	PC1	C3C-C3D-C3E-C3F
51	M	505	CDL	OB5-CB3-CB4-CB6
51	V	203	CDL	OB5-CB3-CB4-CB6
51	Y	201	CDL	OB5-CB3-CB4-CB6
51	W	201	CDL	CB2-C1-CA2-OA2
49	A	201	PC1	O11-C1-C2-O21
50	M	502	3PE	O11-C1-C2-O21
50	V	201	3PE	C26-C27-C28-C29
50	6	203	3PE	C25-C26-C27-C28
50	6	203	3PE	O21-C21-C22-C23
49	9	401	PC1	C3A-C3B-C3C-C3D
51	V	203	CDL	C53-C54-C55-C56
50	M	501	3PE	C35-C36-C37-C38
50	V	201	3PE	C32-C33-C34-C35
51	M	505	CDL	C62-C63-C64-C65
51	V	203	CDL	C20-C21-C22-C23
51	L	1003	CDL	C1-CB2-OB2-PB2
51	M	505	CDL	C11-C12-C13-C14
51	W	201	CDL	C12-C13-C14-C15
51	L	1003	CDL	C55-C56-C57-C58
49	L	1002	PC1	C27-C28-C29-C2A
50	A	202	3PE	O11-C1-C2-C3
50	M	502	3PE	C39-C3A-C3B-C3C
51	V	203	CDL	C78-C79-C80-C81
49	9	401	PC1	C29-C2A-C2B-C2C
51	V	203	CDL	C55-C56-C57-C58
51	L	1003	CDL	C78-C79-C80-C81
49	M	504	PC1	C23-C24-C25-C26
51	L	1003	CDL	C82-C83-C84-C85
49	M	503	PC1	C11-C12-N-C14
51	L	1003	CDL	C79-C80-C81-C82
51	M	505	CDL	C53-C54-C55-C56
49	9	401	PC1	C3-C2-O21-C21
49	L	1002	PC1	C1-C2-O21-C21
50	L	1004	3PE	C1-C2-O21-C21
56	s	201	MYR	C11-C10-C9-C8
49	9	401	PC1	C39-C3A-C3B-C3C
52	g	201	ZMP	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
51	V	203	CDL	CA4-CA3-OA5-PA1
51	o	502	CDL	CB4-CB3-OB5-PB2
49	M	504	PC1	C29-C2A-C2B-C2C
49	L	1002	PC1	C3D-C3E-C3F-C3G
51	M	505	CDL	OA6-CA4-CA6-OA8
51	Y	201	CDL	C72-C73-C74-C75
49	L	1002	PC1	C21-C22-C23-C24
50	M	501	3PE	C36-C37-C38-C39
51	W	201	CDL	CA5-C11-C12-C13
54	d	401	NDP	C2B-O2B-P2B-O1X
51	L	1003	CDL	C40-C41-C42-C43
51	V	204	CDL	C72-C73-C74-C75
49	6	202	PC1	O11-C1-C2-O21
49	M	504	PC1	C24-C25-C26-C27
51	W	201	CDL	C53-C54-C55-C56
49	A	201	PC1	O21-C21-C22-C23
50	A	202	3PE	C3C-C3D-C3E-C3F
49	L	1002	PC1	C23-C24-C25-C26
46	1	501	FMN	C1'-C2'-C3'-O3'
51	W	201	CDL	OA6-CA4-CA6-OA8
51	Y	201	CDL	C80-C81-C82-C83
51	V	204	CDL	C1-CA2-OA2-PA1
50	H	401	3PE	C2F-C2G-C2H-C2I
50	N	401	3PE	C2C-C2D-C2E-C2F
51	V	203	CDL	C13-C14-C15-C16
51	z	101	CDL	C52-C53-C54-C55
50	N	401	3PE	C3-C2-O21-C21
49	M	504	PC1	C32-C33-C34-C35
50	K	101	3PE	C31-C32-C33-C34
49	M	503	PC1	C2D-C2E-C2F-C2G
49	M	504	PC1	C2D-C2E-C2F-C2G
51	Y	201	CDL	C57-C58-C59-C60
50	K	101	3PE	C23-C24-C25-C26
49	M	503	PC1	C11-C12-N-C13
49	M	503	PC1	C11-C12-N-C15
50	N	401	3PE	C1-C2-C3-O31
49	9	401	PC1	C22-C23-C24-C25
51	V	204	CDL	C31-C32-C33-C34
50	H	401	3PE	C12-C11-O13-P
50	N	401	3PE	C34-C35-C36-C37
50	o	501	3PE	C22-C23-C24-C25
49	6	202	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
51	V	203	CDL	C24-C25-C26-C27
50	M	501	3PE	O21-C2-C3-O31
51	L	1003	CDL	OA6-CA4-CA6-OA8
49	6	202	PC1	O11-C1-C2-C3
51	o	502	CDL	OB5-CB3-CB4-CB6
50	N	401	3PE	C27-C28-C29-C2A
51	W	201	CDL	C19-C20-C21-C22
49	M	504	PC1	O21-C21-C22-C23
51	V	204	CDL	C52-C51-CB5-OB6
50	6	203	3PE	C29-C2A-C2B-C2C
50	L	1001	3PE	O21-C21-C22-C23
51	V	204	CDL	C72-C71-CB7-OB8
51	z	101	CDL	C32-C31-CA7-OA8
55	k	501	AMP	O4'-C1'-N9-C8
51	L	1003	CDL	C77-C78-C79-C80
51	Y	201	CDL	C12-C11-CA5-OA6
50	N	401	3PE	C22-C23-C24-C25
51	W	201	CDL	C14-C15-C16-C17
50	M	501	3PE	O21-C21-C22-C23
51	V	204	CDL	C32-C31-CA7-OA8
49	M	504	PC1	C37-C38-C39-C3A
49	9	401	PC1	C3D-C3E-C3F-C3G
49	M	504	PC1	O21-C2-C3-O31
51	V	203	CDL	OA6-CA4-CA6-OA8
51	o	502	CDL	OB6-CB4-CB6-OB8
50	M	502	3PE	O31-C31-C32-C33
50	p	201	3PE	C25-C26-C27-C28
52	X	101	ZMP	C20-C18-C21-O5
49	M	503	PC1	O31-C31-C32-C33
50	p	201	3PE	O21-C21-C22-C23
51	V	203	CDL	C32-C31-CA7-OA8
56	s	201	MYR	C9-C10-C11-C12
51	M	505	CDL	CB3-CB4-OB6-CB5
50	H	401	3PE	C36-C37-C38-C39
49	9	401	PC1	C2D-C2E-C2F-C2G
50	H	401	3PE	C3C-C3D-C3E-C3F
49	9	401	PC1	C3F-C3G-C3H-C3I
50	6	203	3PE	C33-C34-C35-C36
51	V	203	CDL	C32-C31-CA7-OA9
51	M	505	CDL	OA5-CA3-CA4-OA6
51	z	101	CDL	C52-C51-CB5-OB6
51	M	505	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
51	V	204	CDL	C52-C51-CB5-OB7
50	M	501	3PE	C33-C34-C35-C36
50	p	201	3PE	C26-C27-C28-C29
51	V	204	CDL	C72-C71-CB7-OB9
49	L	1002	PC1	C39-C3A-C3B-C3C
51	o	502	CDL	C52-C51-CB5-OB6
50	M	501	3PE	O22-C21-C22-C23
50	M	501	3PE	O31-C31-C32-C33
50	M	502	3PE	O32-C31-C32-C33
50	L	1001	3PE	O22-C21-C22-C23
51	V	204	CDL	C32-C31-CA7-OA9
51	M	505	CDL	C75-C76-C77-C78
51	V	204	CDL	C13-C14-C15-C16
52	g	201	ZMP	N2-C16-C17-O4
50	p	201	3PE	O22-C21-C22-C23
51	V	204	CDL	C1-CB2-OB2-PB2
49	9	401	PC1	O31-C31-C32-C33
51	M	505	CDL	C72-C71-CB7-OB8
50	6	203	3PE	C3D-C3E-C3F-C3G
51	V	204	CDL	C23-C24-C25-C26
52	X	101	ZMP	C17-C18-C21-O5
50	A	202	3PE	O21-C21-C22-C23
49	M	503	PC1	O32-C31-C32-C33
51	z	101	CDL	C32-C31-CA7-OA9
51	Y	201	CDL	C12-C11-CA5-OA7
50	V	201	3PE	O21-C21-C22-C23
51	W	201	CDL	C32-C31-CA7-OA8
51	o	502	CDL	C72-C71-CB7-OB8
49	9	401	PC1	O32-C31-C32-C33
50	H	401	3PE	C29-C2A-C2B-C2C
51	o	502	CDL	C72-C73-C74-C75
50	H	401	3PE	O31-C31-C32-C33
51	o	502	CDL	C72-C71-CB7-OB9
51	Y	201	CDL	C12-C13-C14-C15

There are no ring outliers.

28 monomers are involved in 82 short contacts:

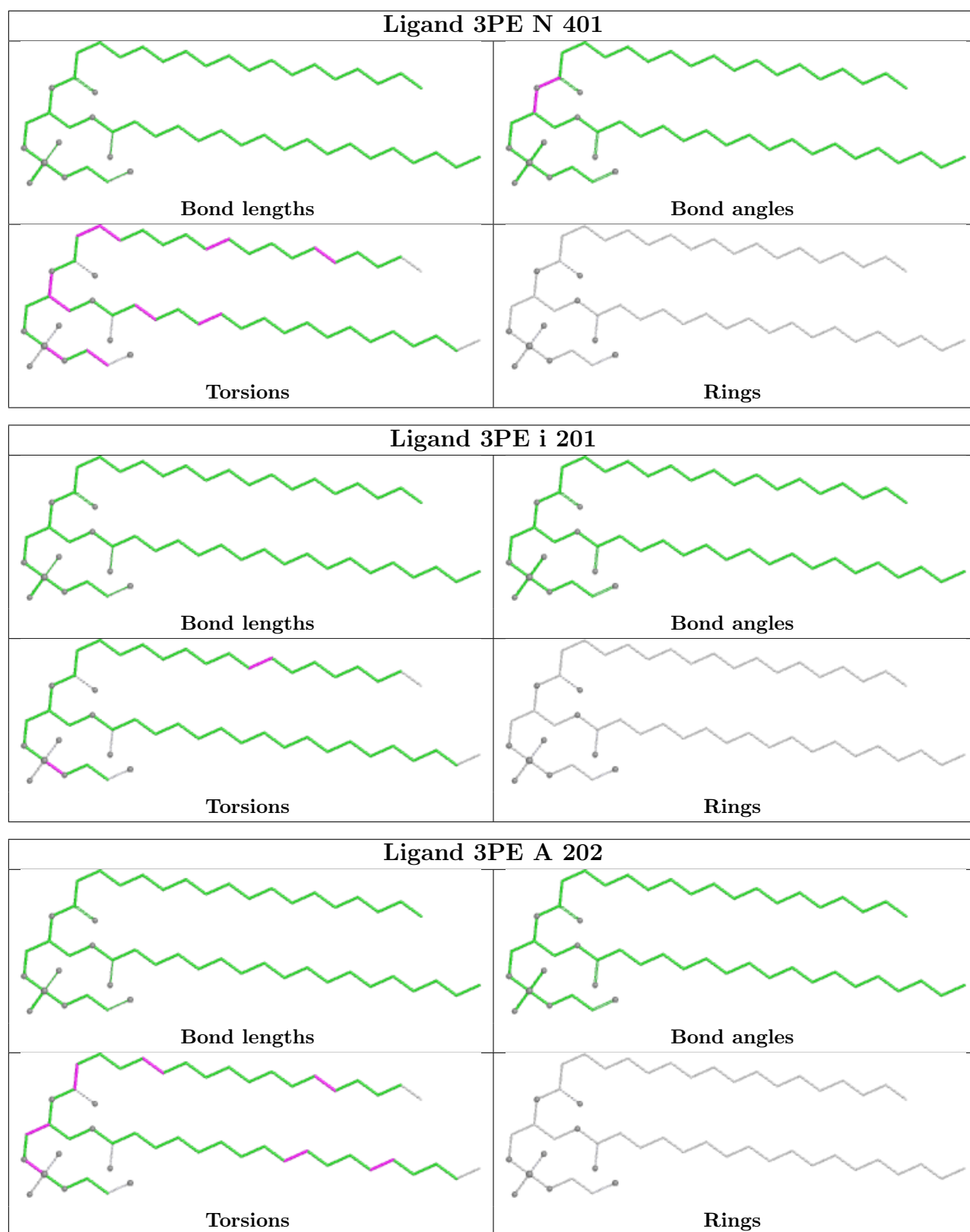
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	i	201	3PE	1	0
50	A	202	3PE	1	0
52	X	101	ZMP	4	0

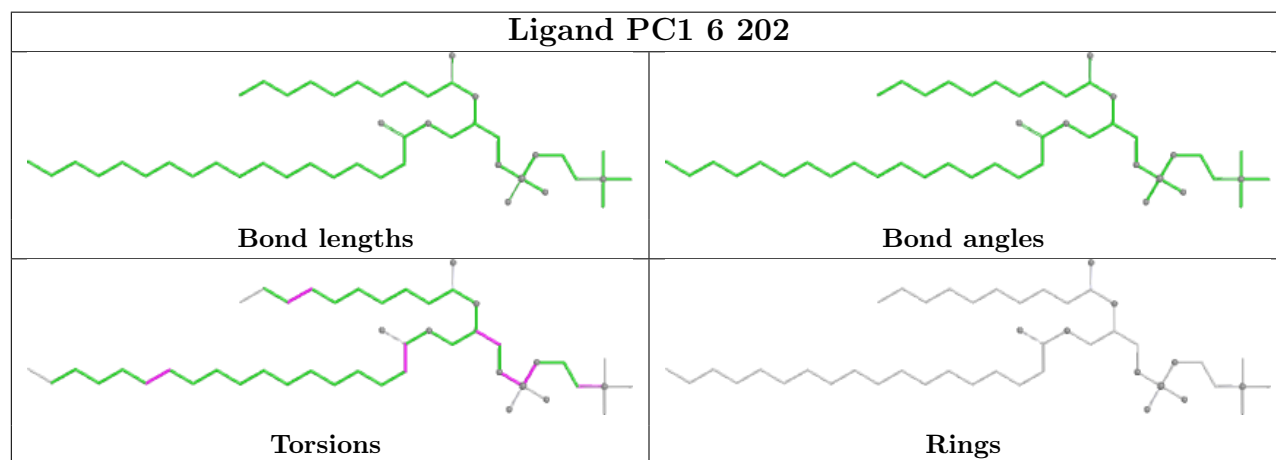
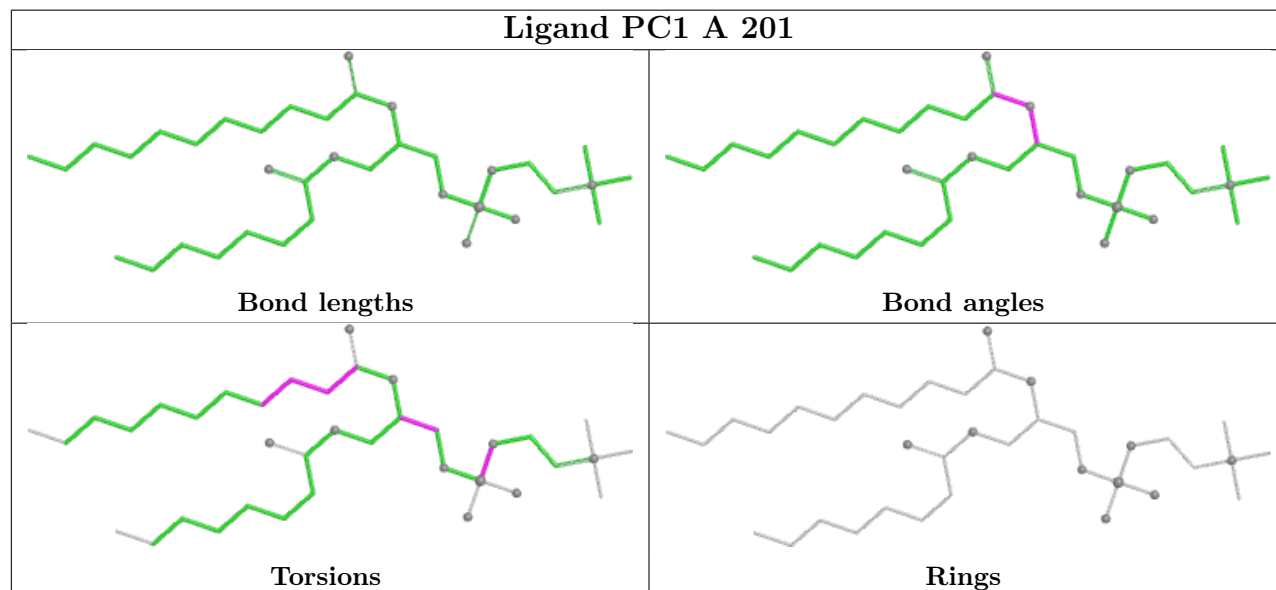
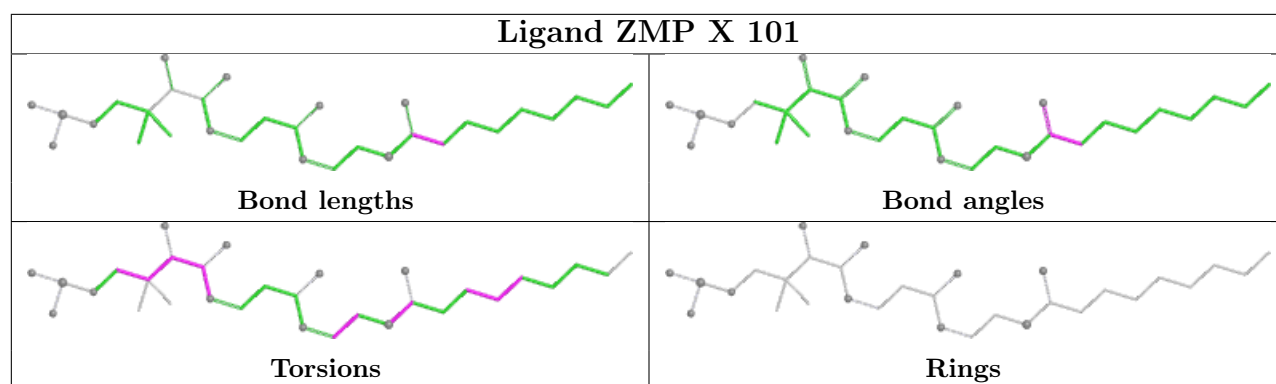
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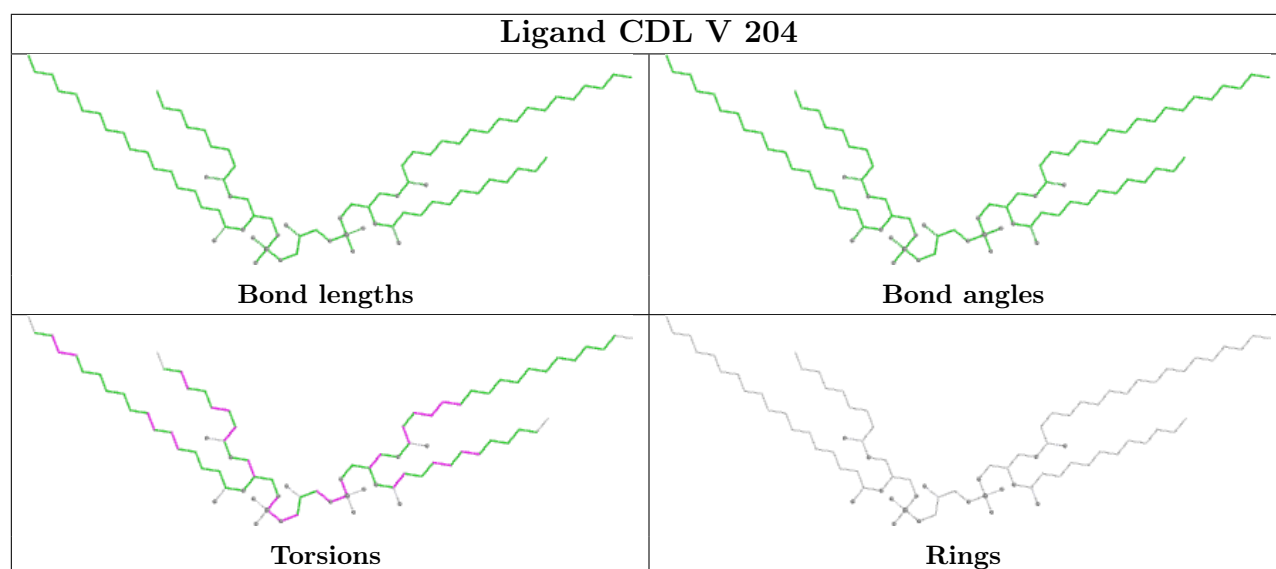
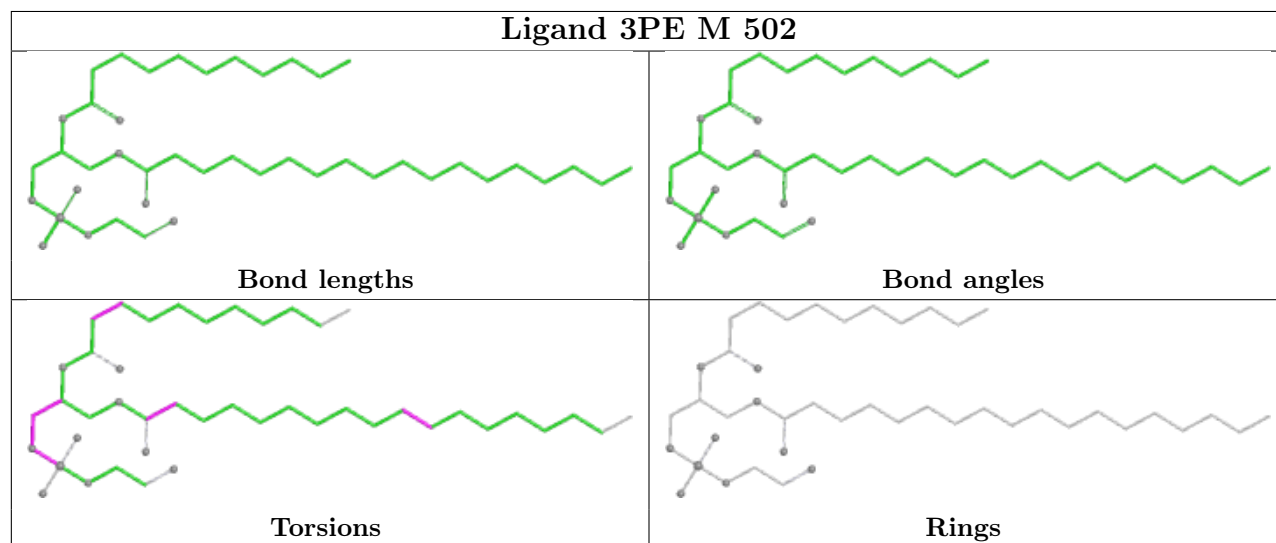
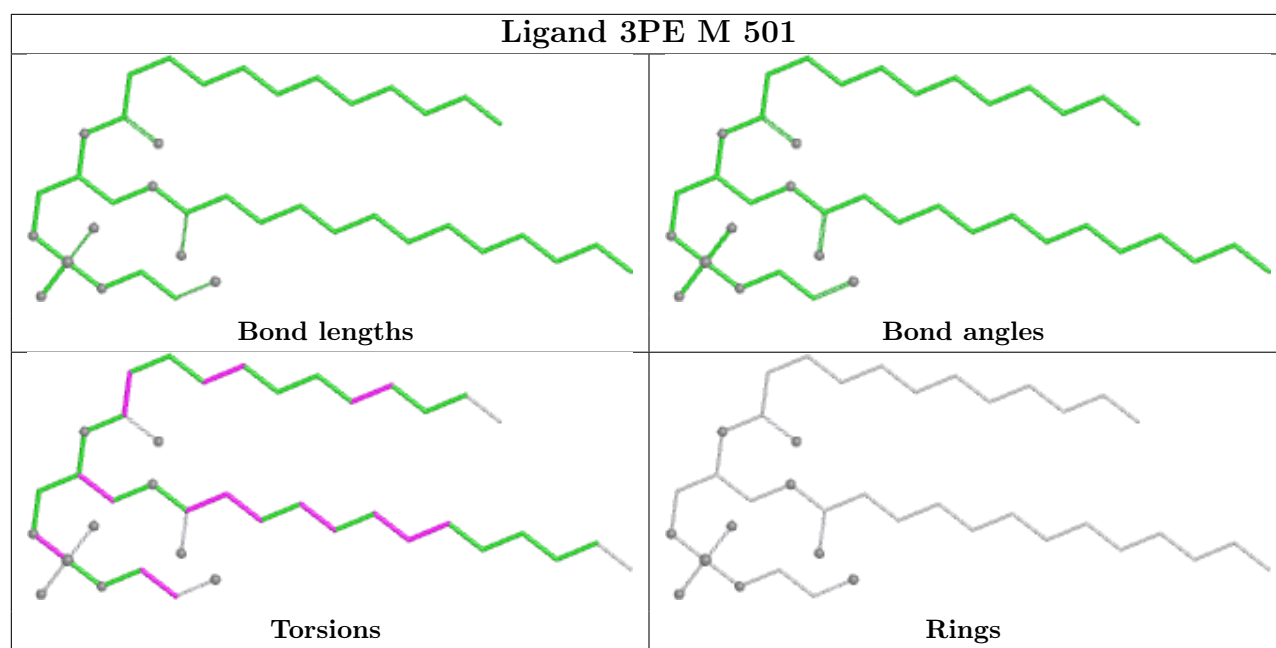
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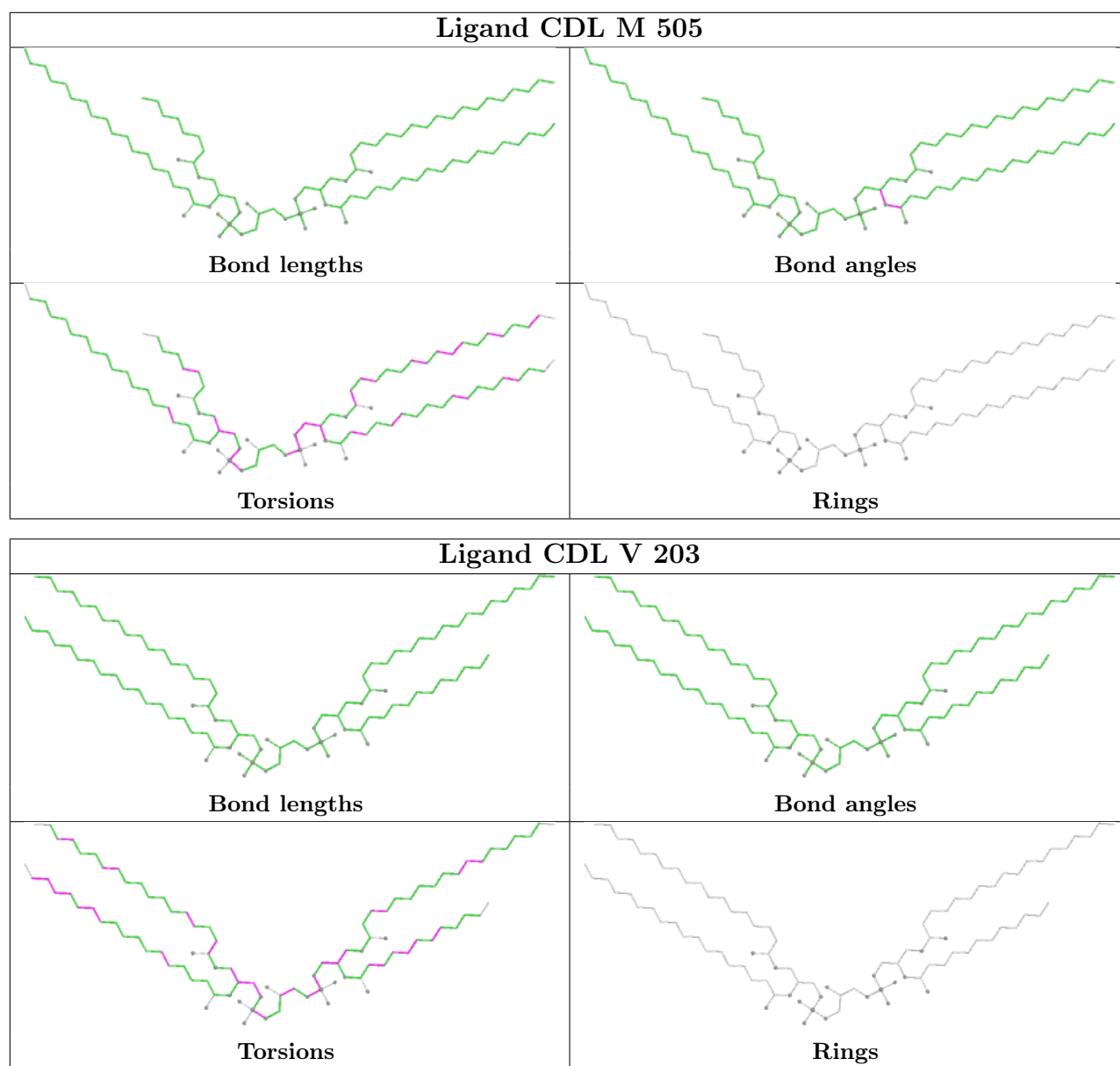
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	A	201	PC1	2	0
45	3	801	SF4	1	0
50	M	501	3PE	3	0
50	M	502	3PE	1	0
51	V	204	CDL	4	0
51	M	505	CDL	3	0
51	V	203	CDL	8	0
51	L	1003	CDL	11	0
50	6	203	3PE	3	0
51	Y	201	CDL	10	0
50	K	101	3PE	1	0
50	H	401	3PE	3	0
45	6	201	SF4	1	0
50	L	1001	3PE	2	0
50	V	202	3PE	3	0
52	g	201	ZMP	2	0
47	2	300	FES	1	0
49	M	503	PC1	7	0
50	V	201	3PE	1	0
51	W	201	CDL	9	0
49	L	1002	PC1	5	0
49	9	401	PC1	2	0
51	o	502	CDL	2	0
49	M	504	PC1	1	0
45	1	500	SF4	2	0

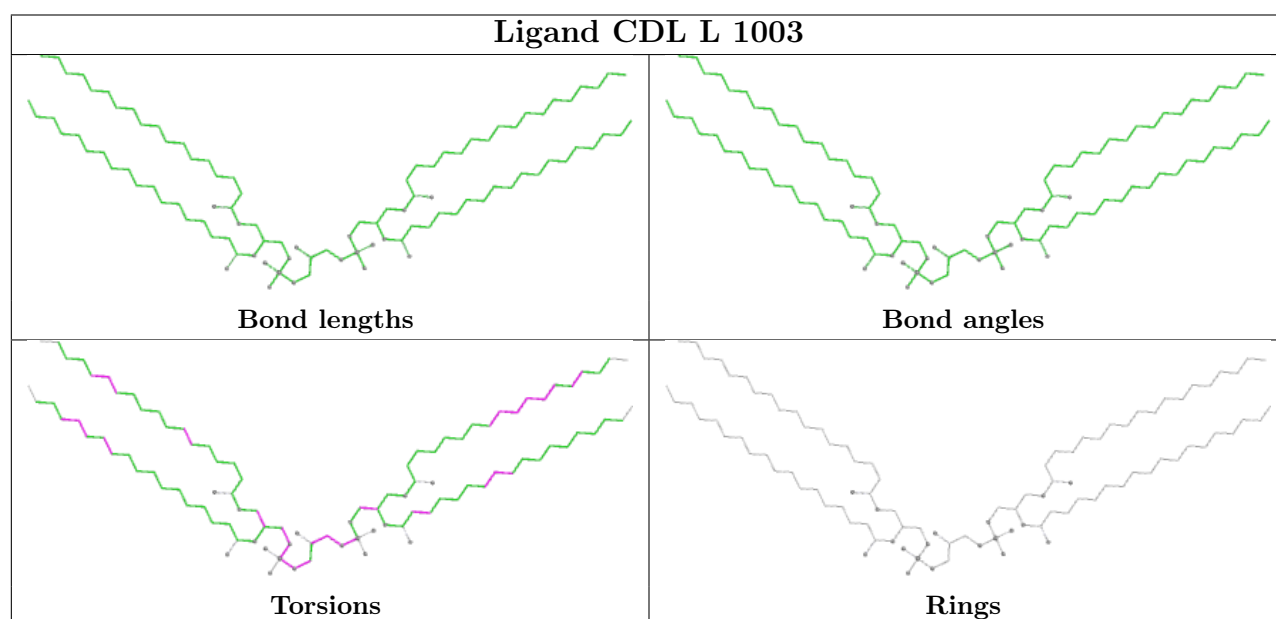
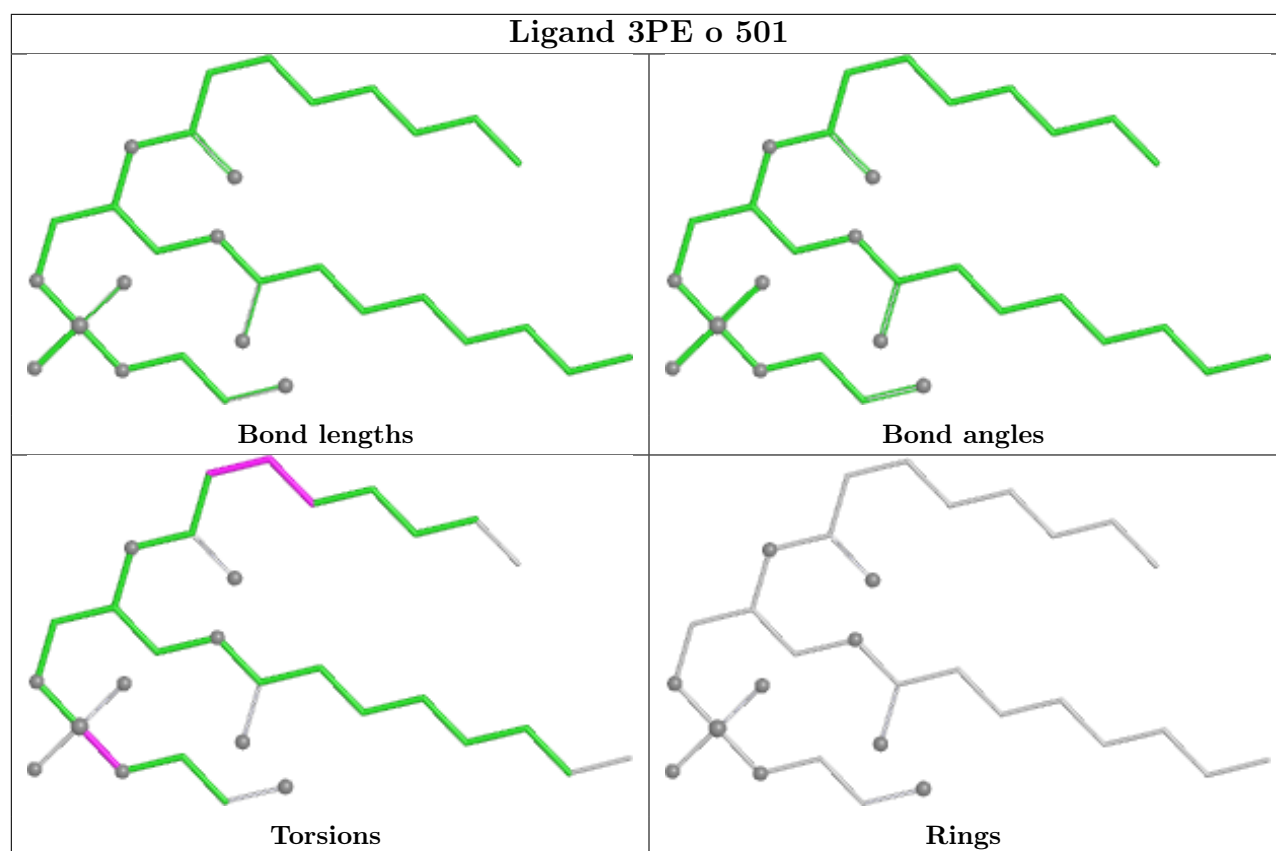
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

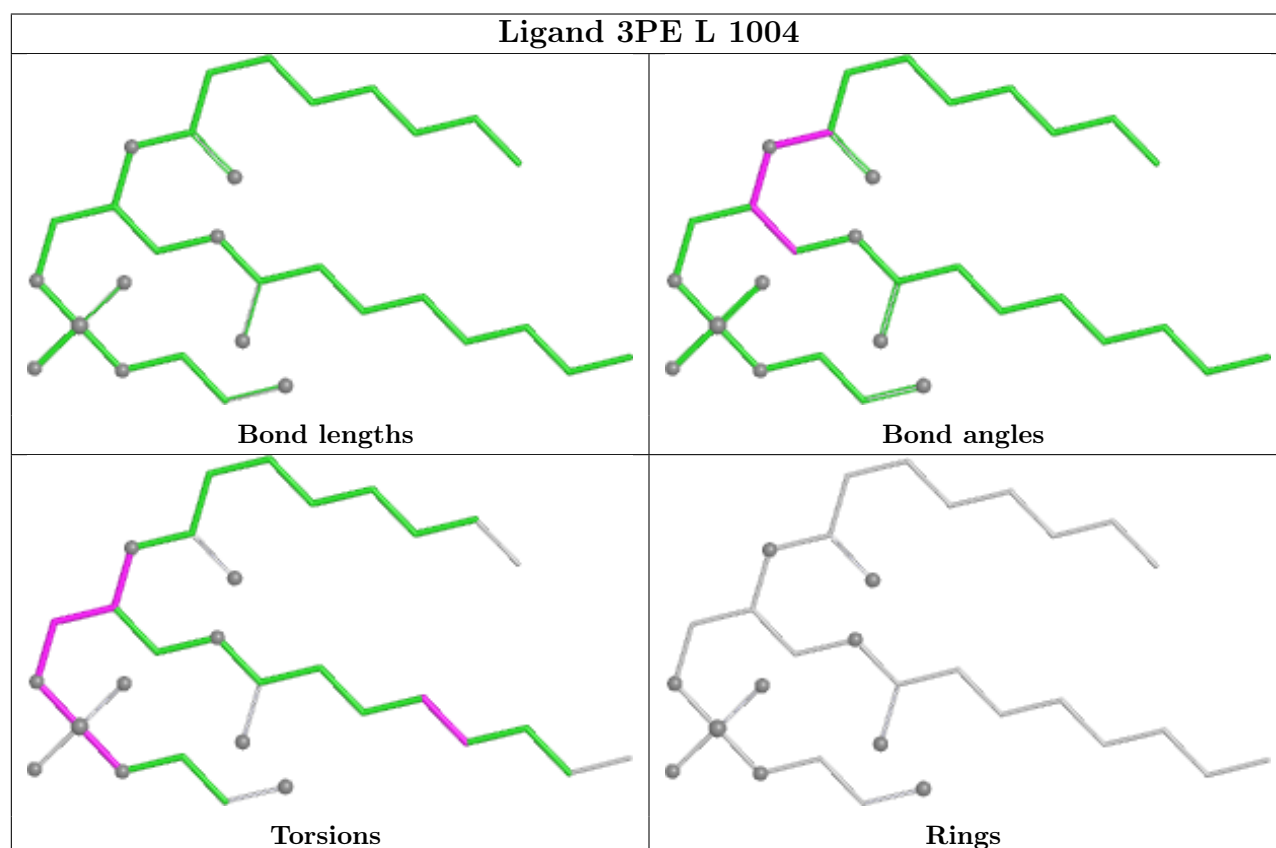
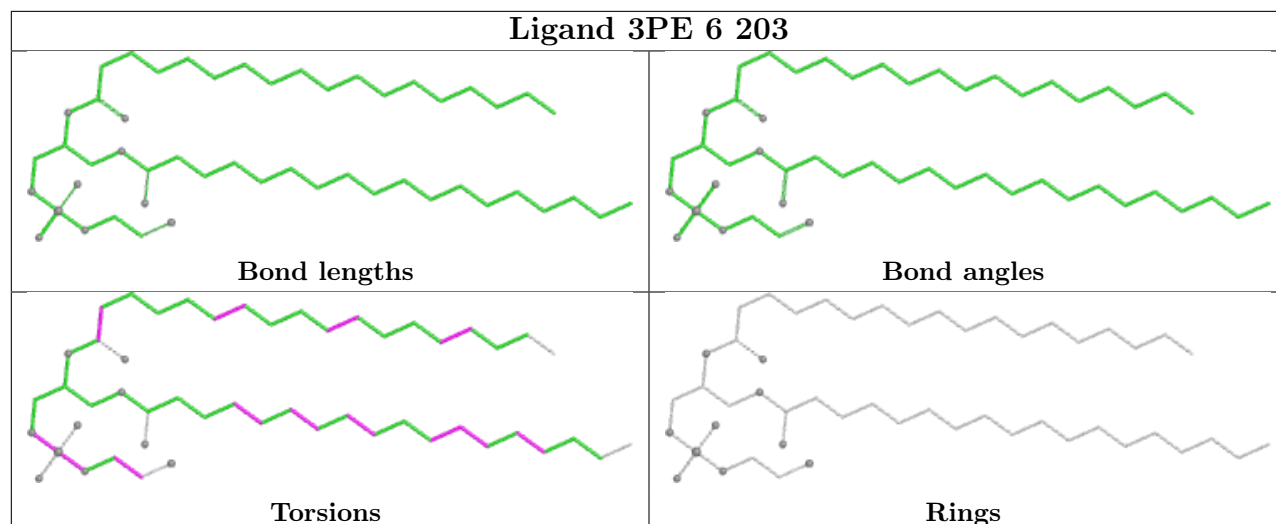


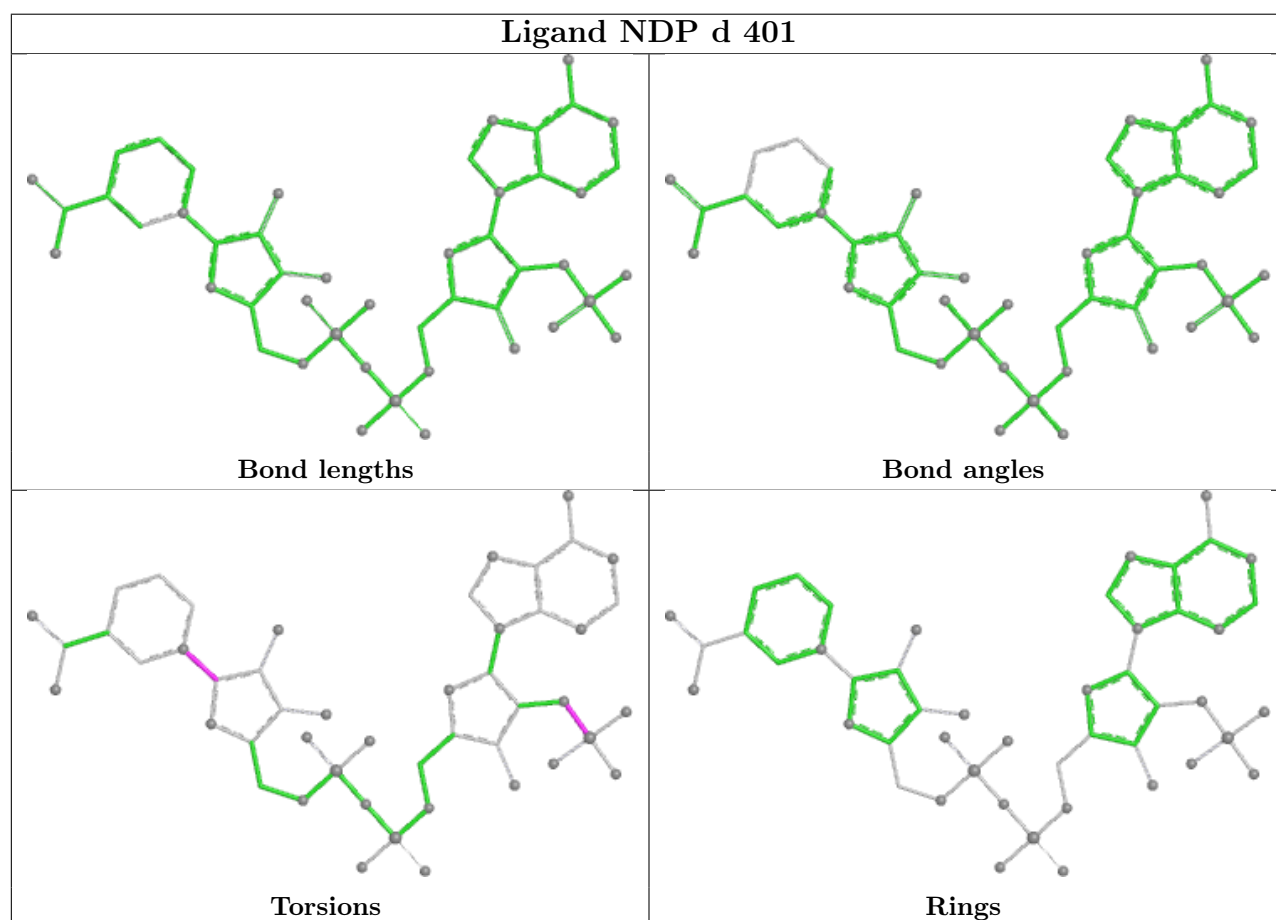
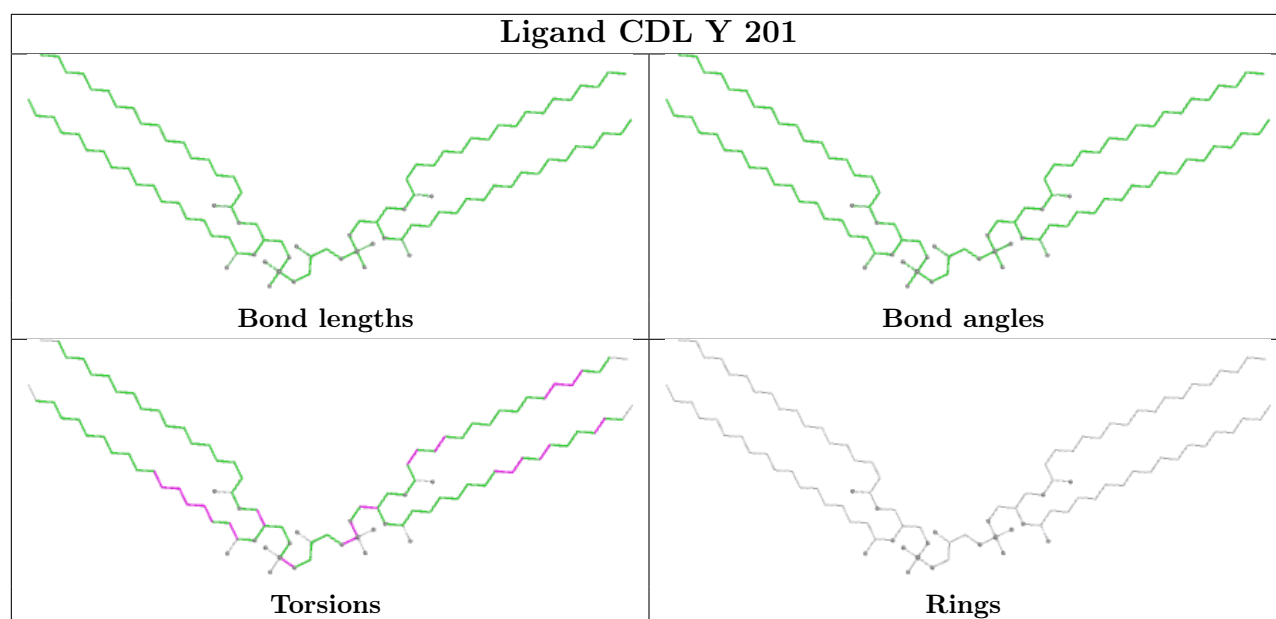


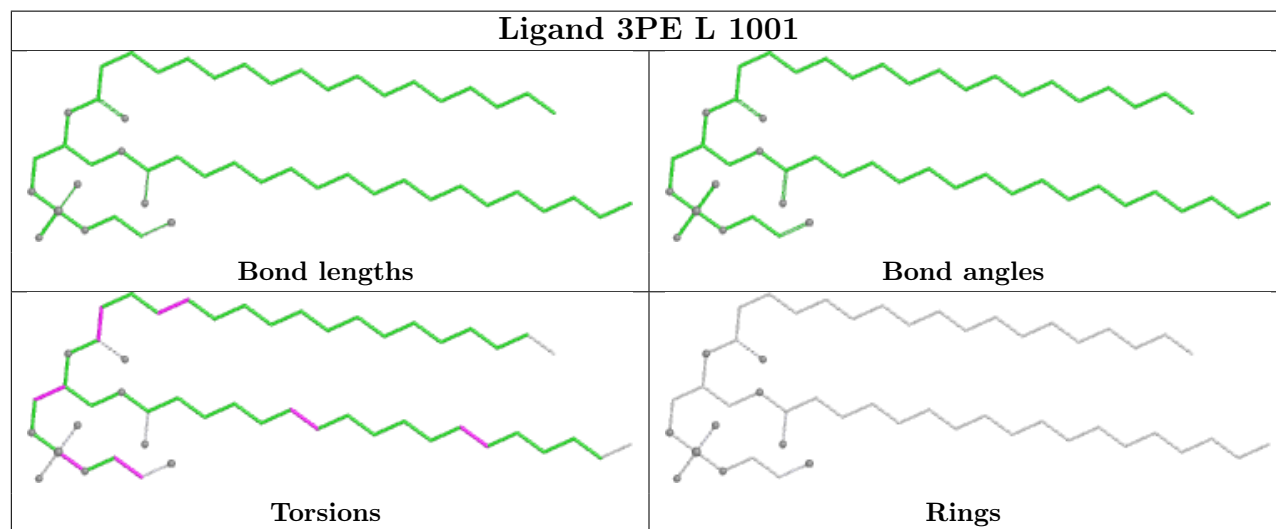
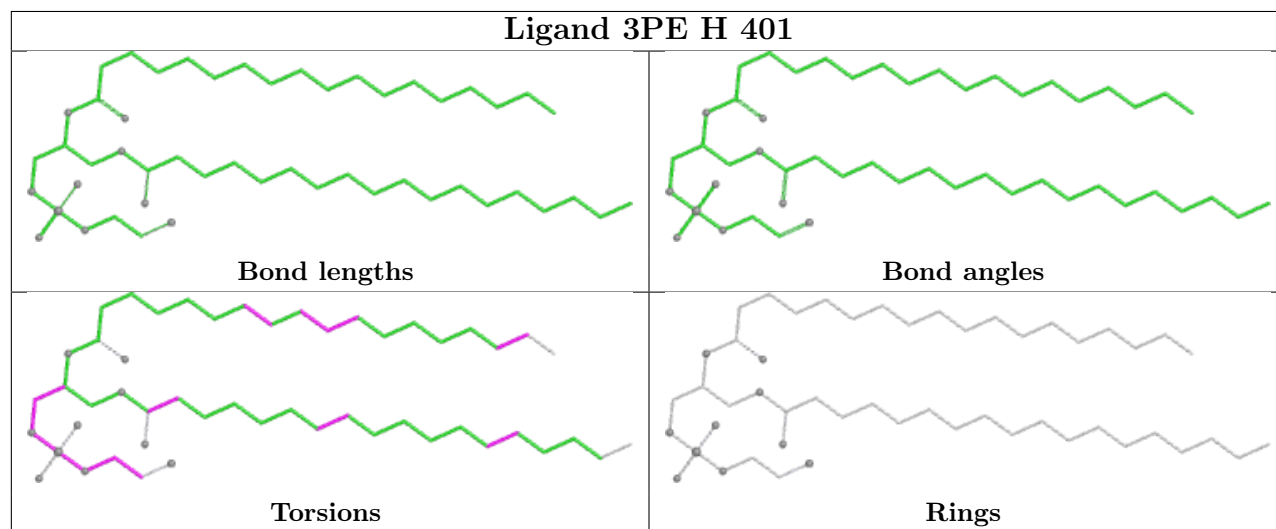
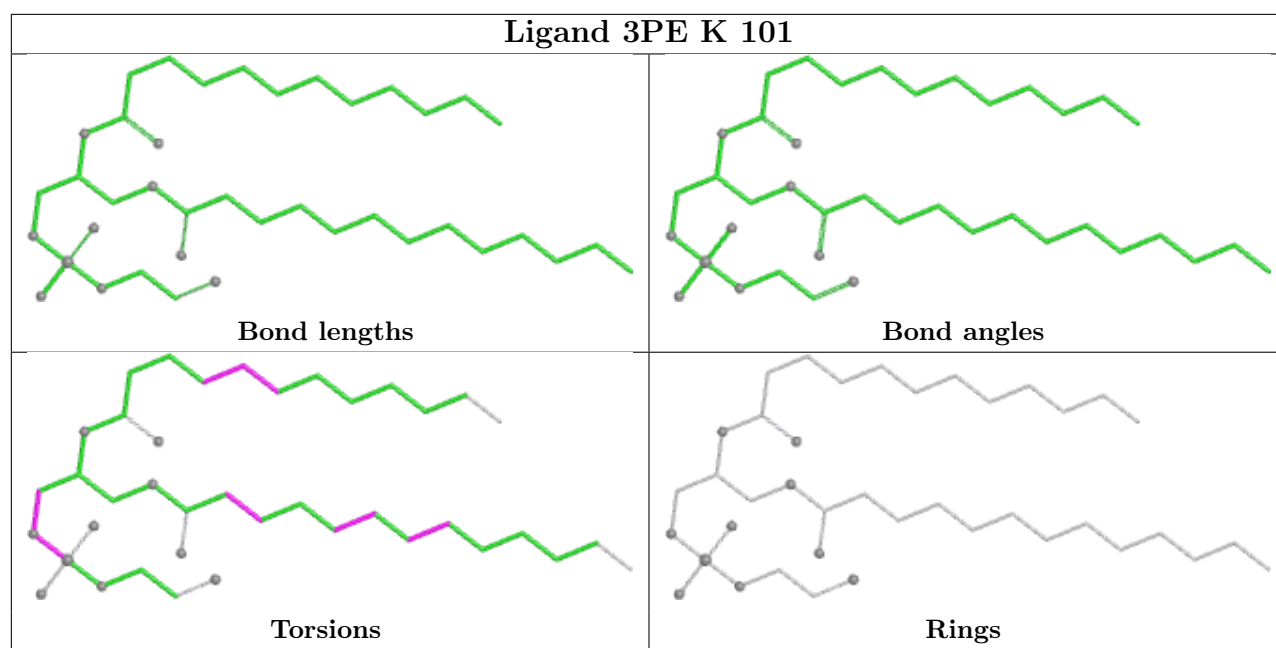


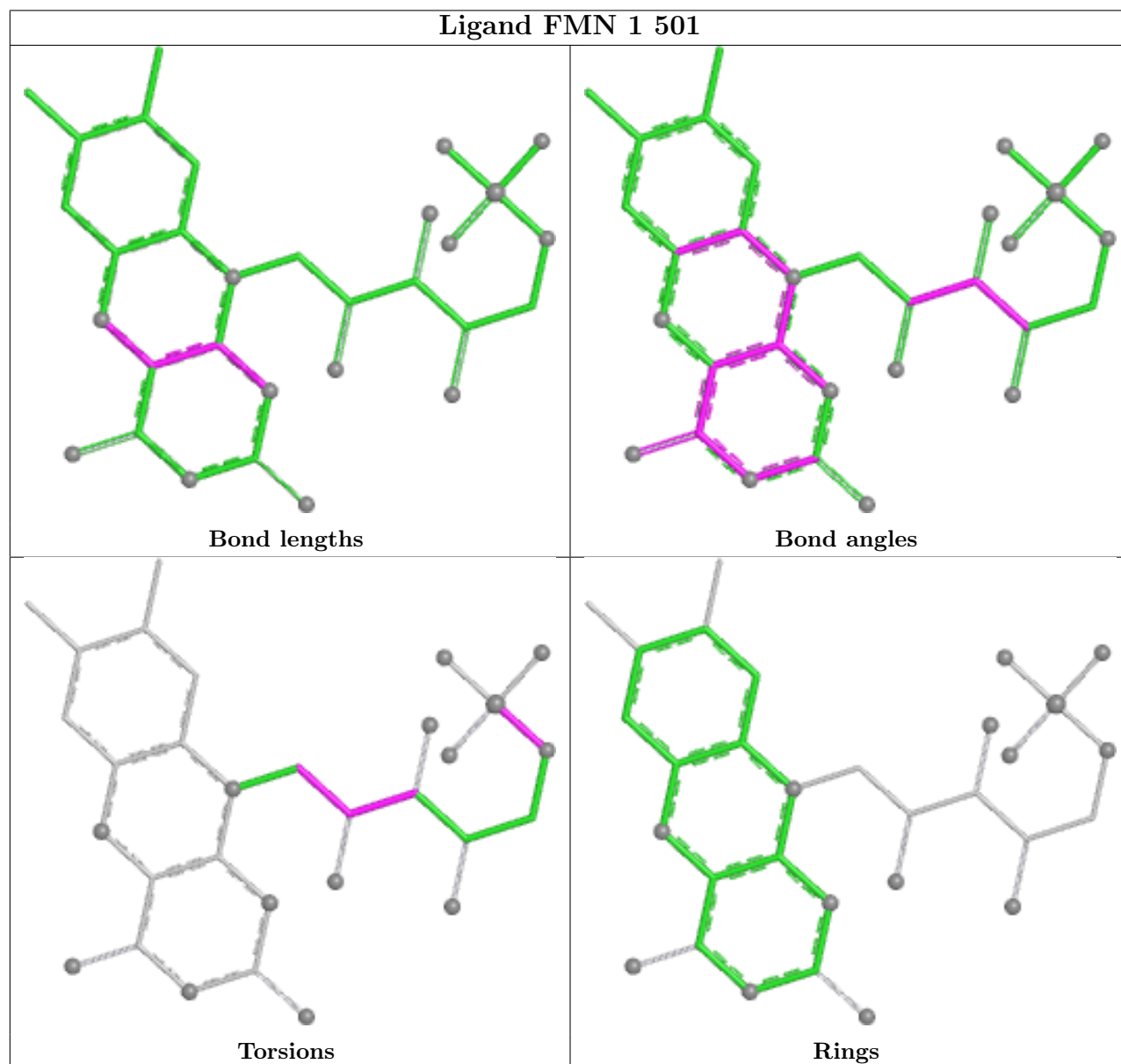
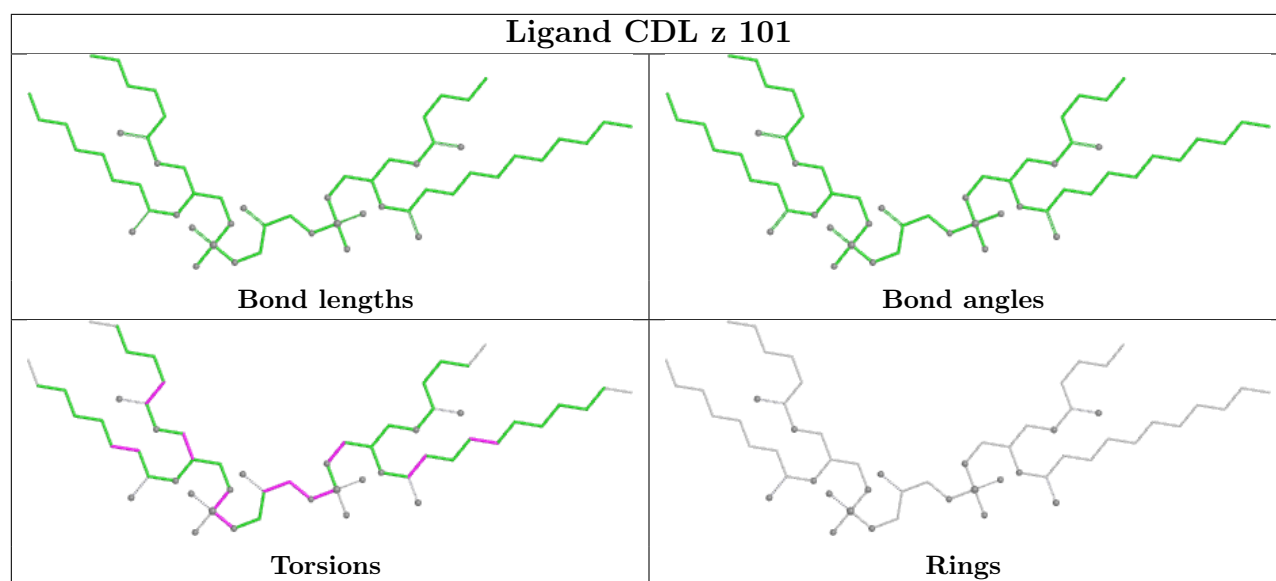


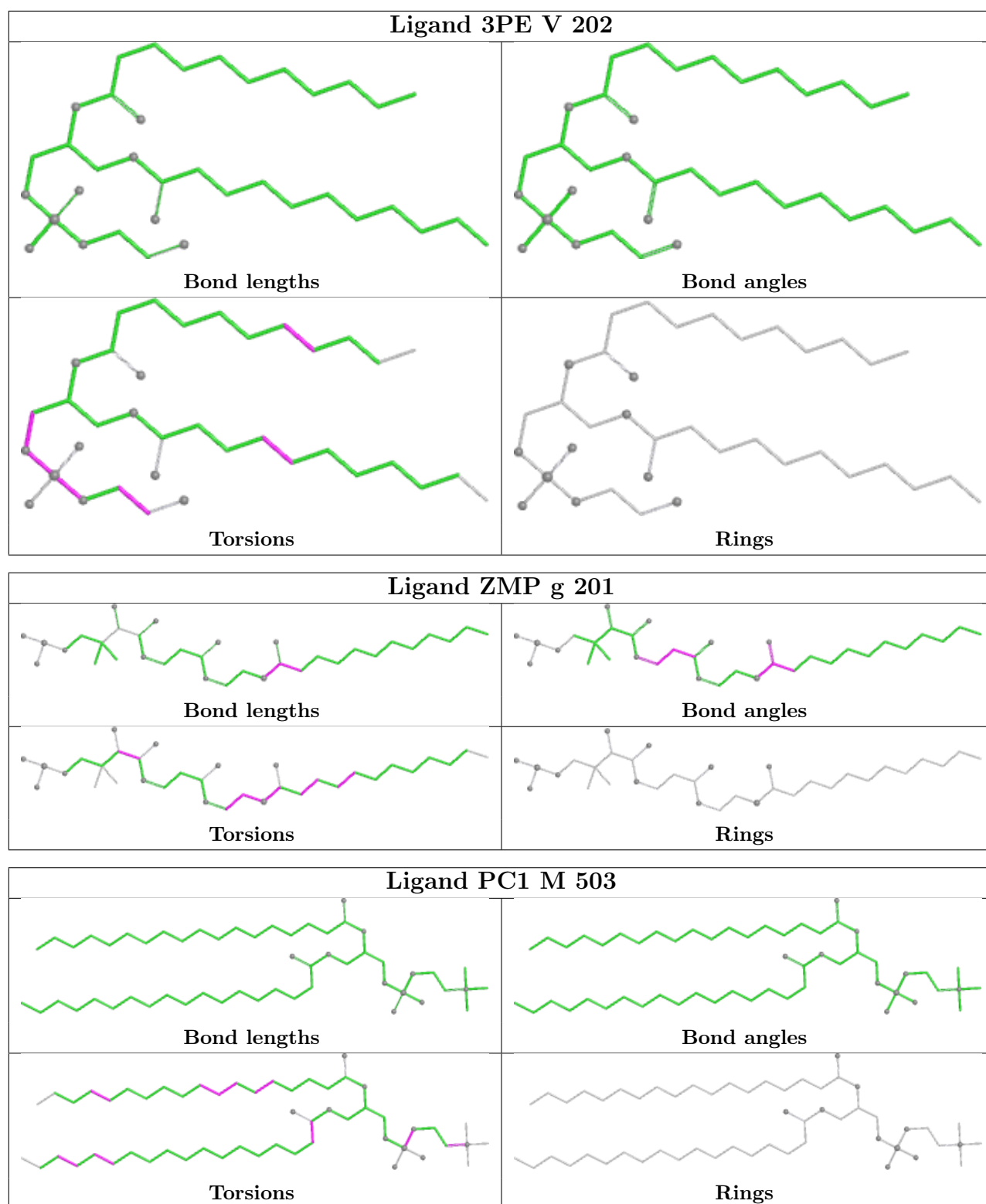


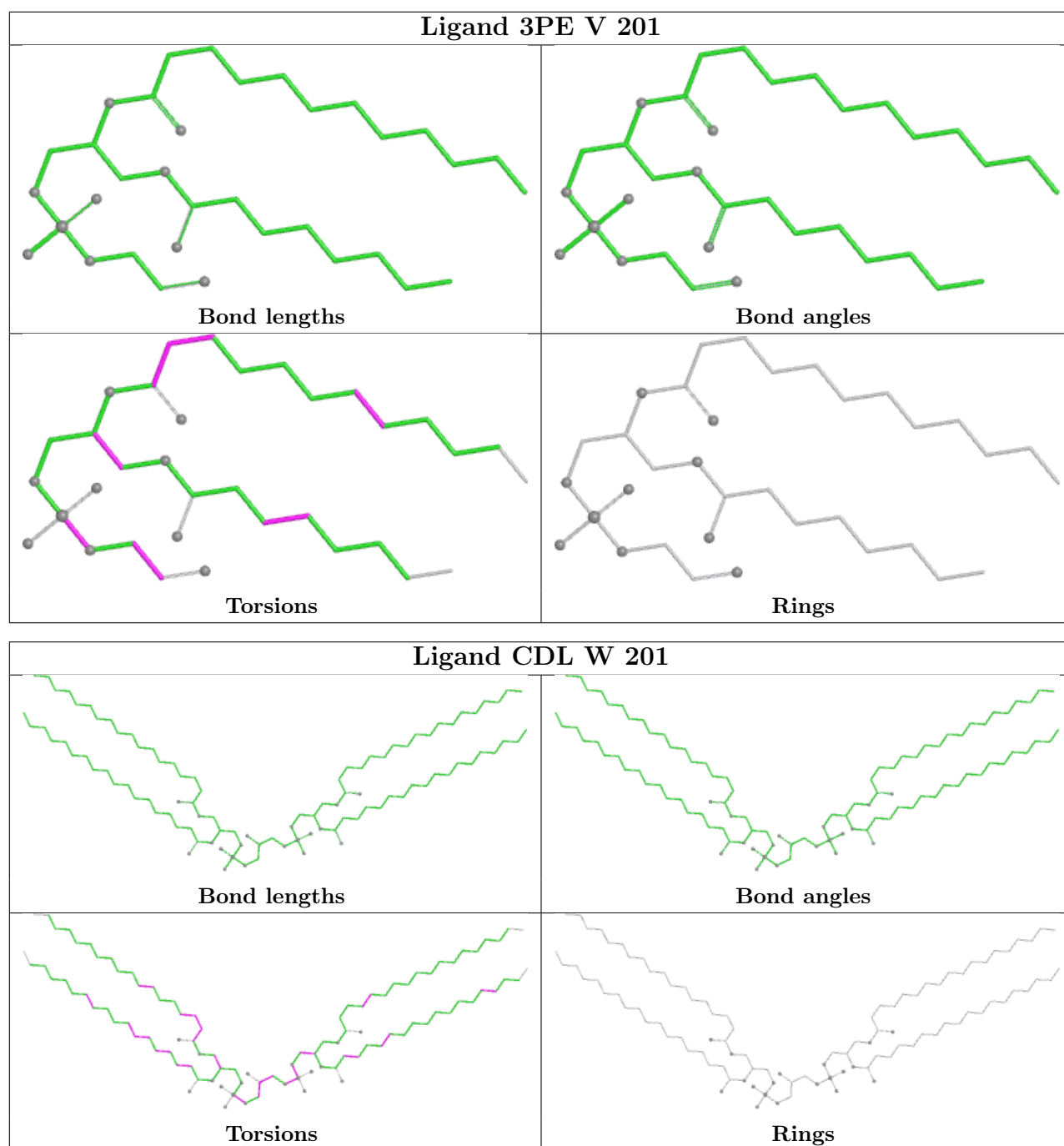


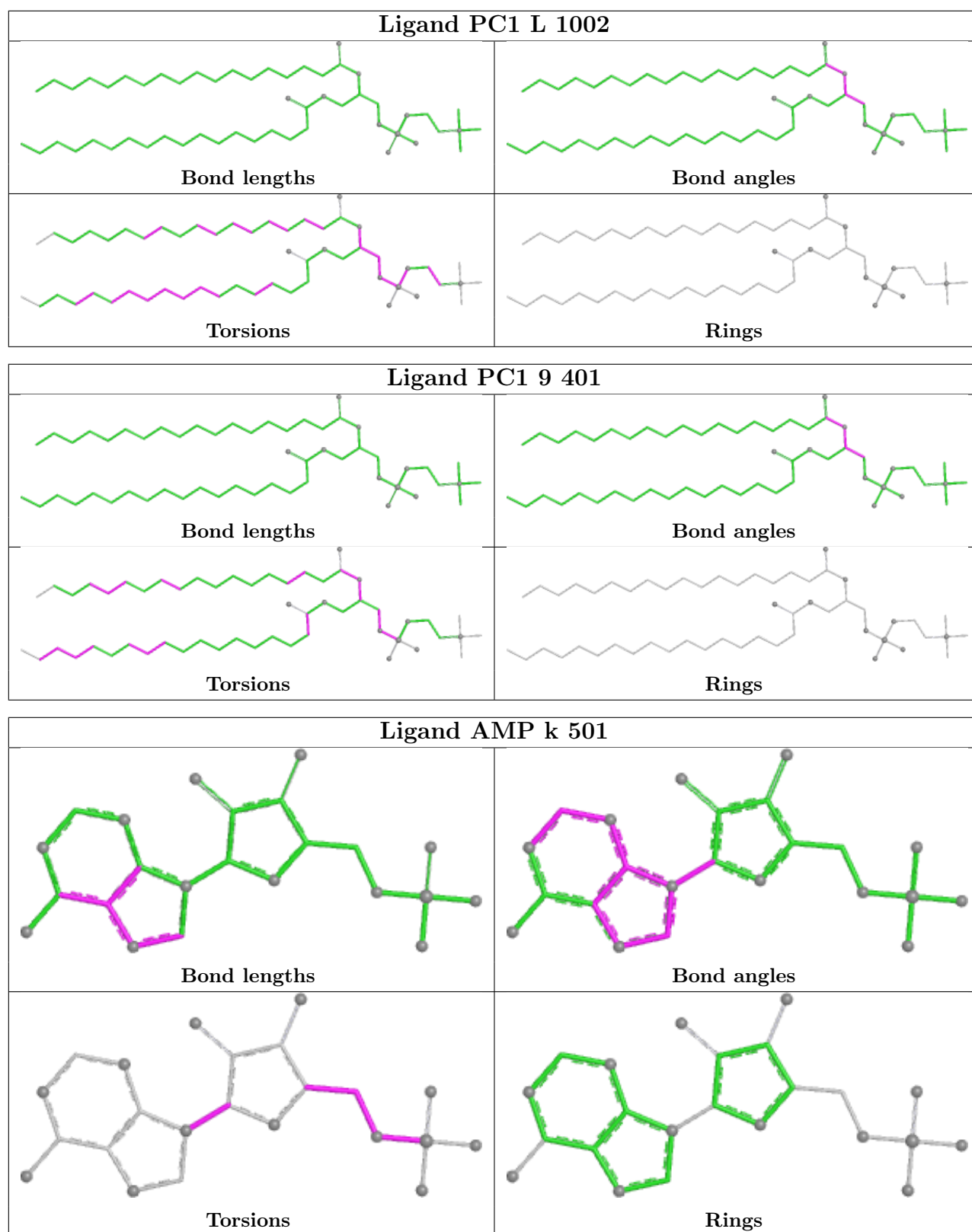


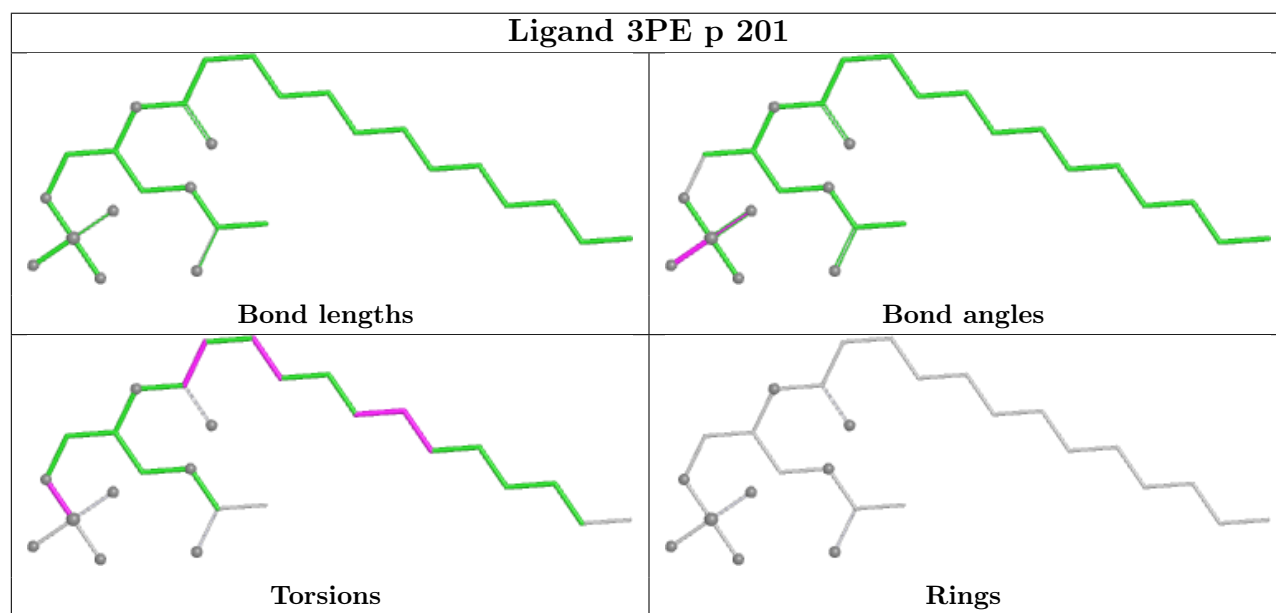
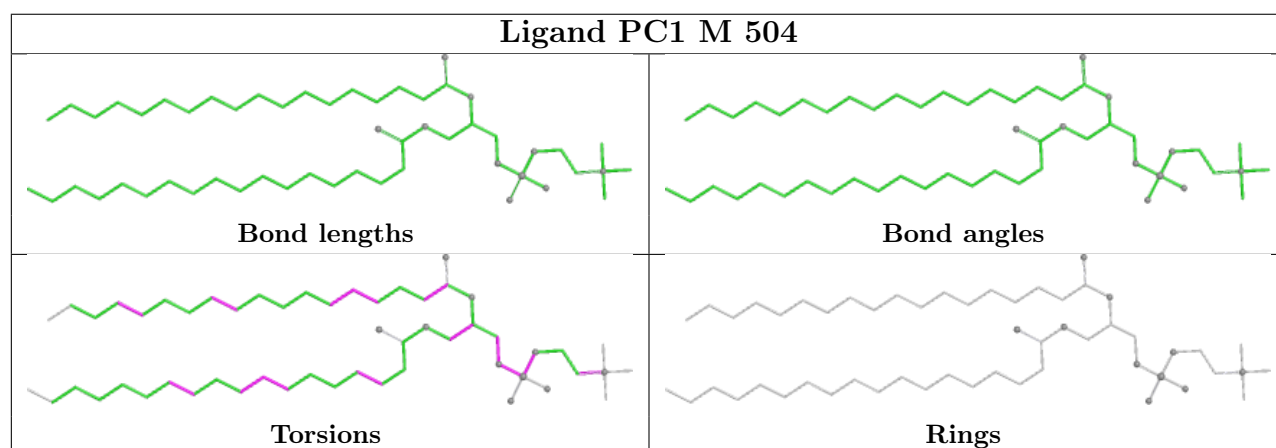
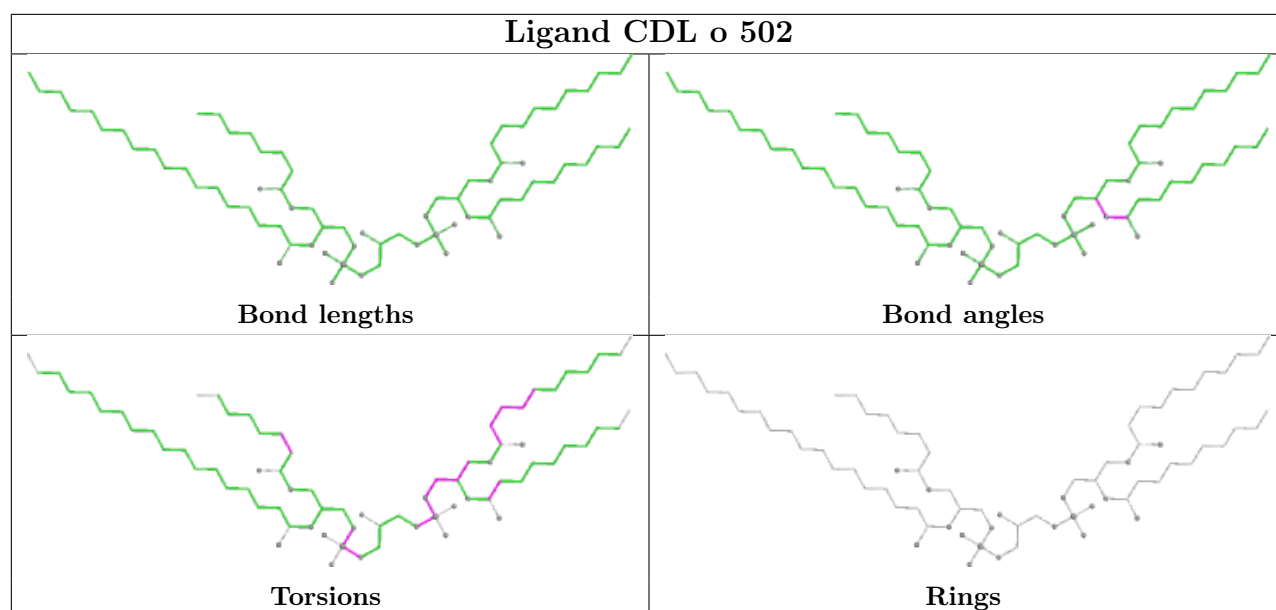












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11259. These allow visual inspection of the internal detail of the map and identification of artifacts.

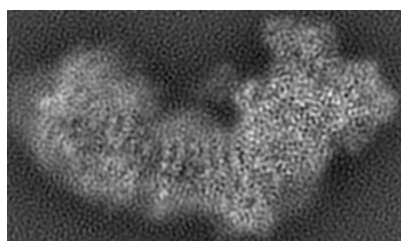
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

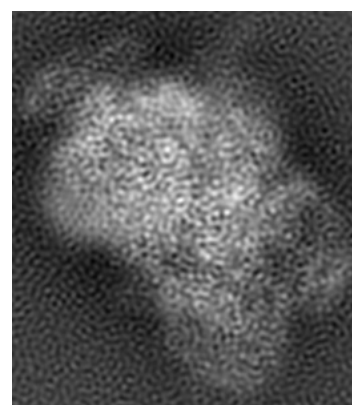
6.1.1 Primary map



X



Y

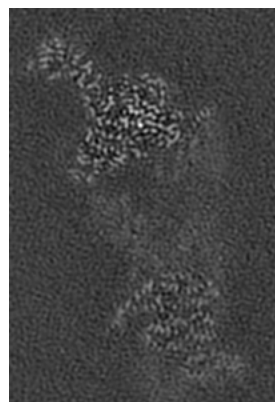


Z

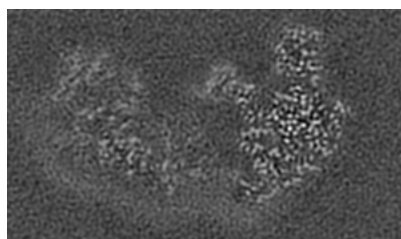
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

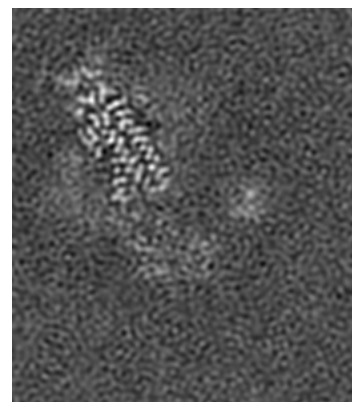
6.2.1 Primary map



X Index: 103



Y Index: 117

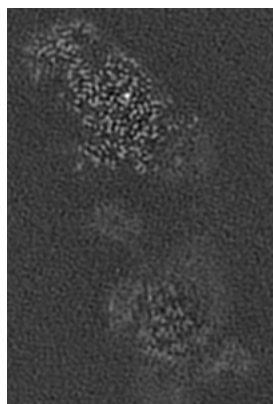


Z Index: 175

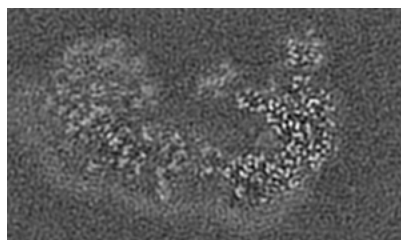
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

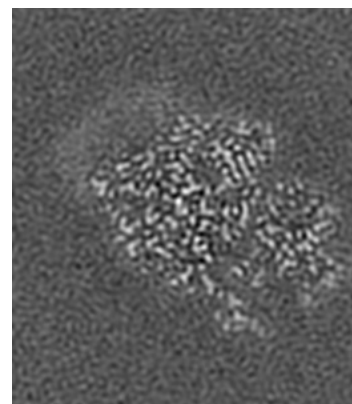
6.3.1 Primary map



X Index: 115



Y Index: 127

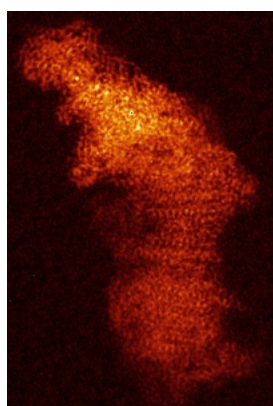


Z Index: 254

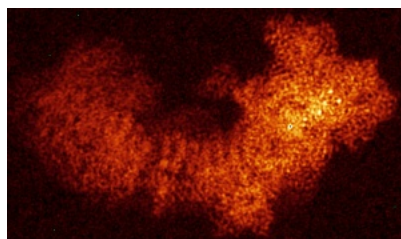
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

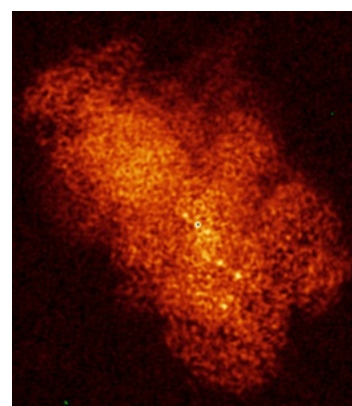
6.4.1 Primary map



X



Y



Z

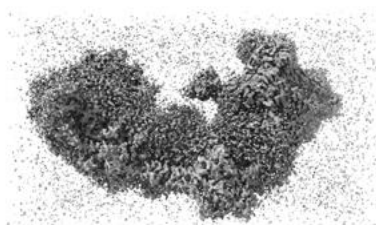
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

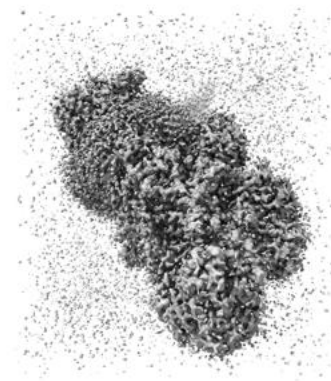
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

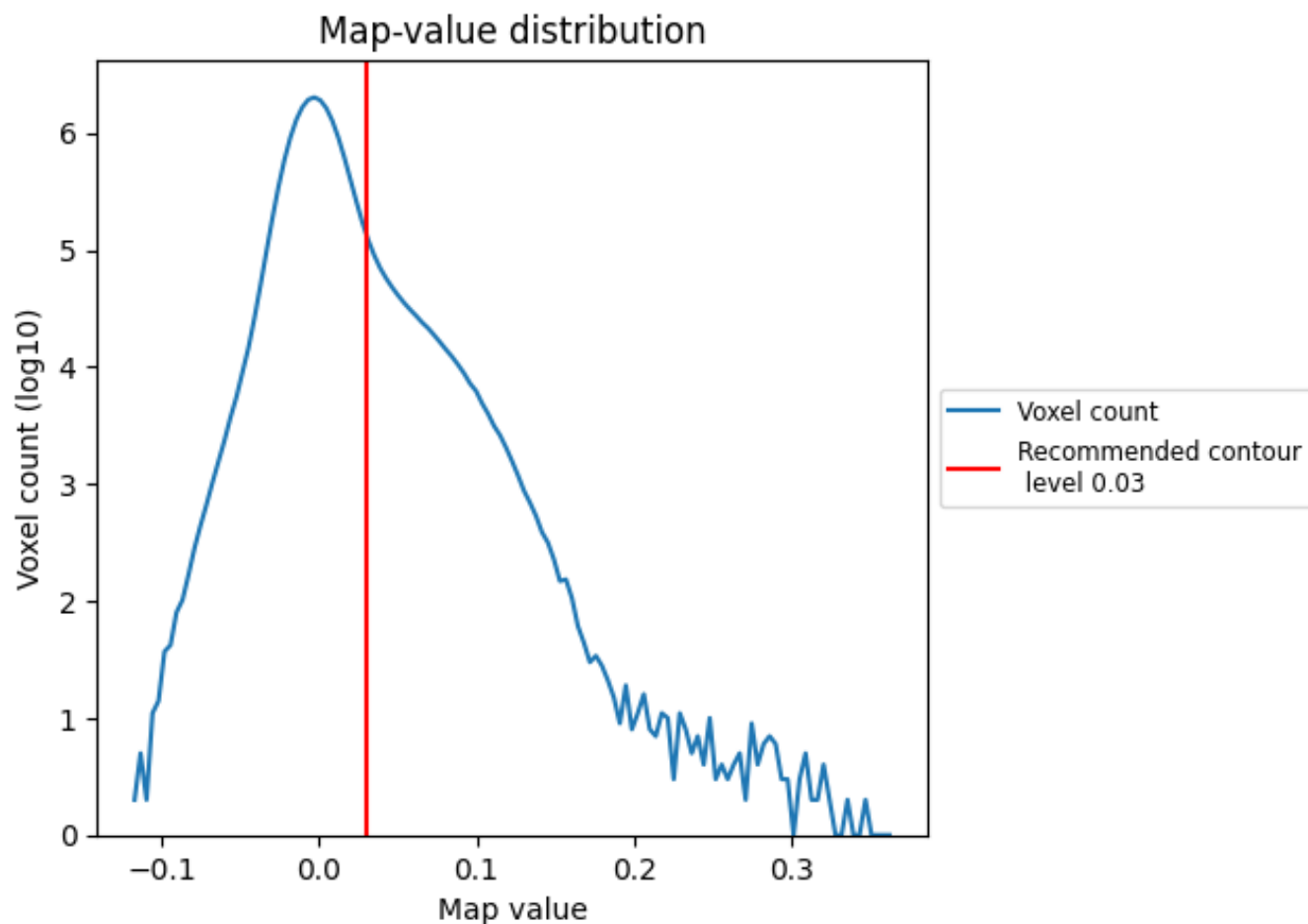
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

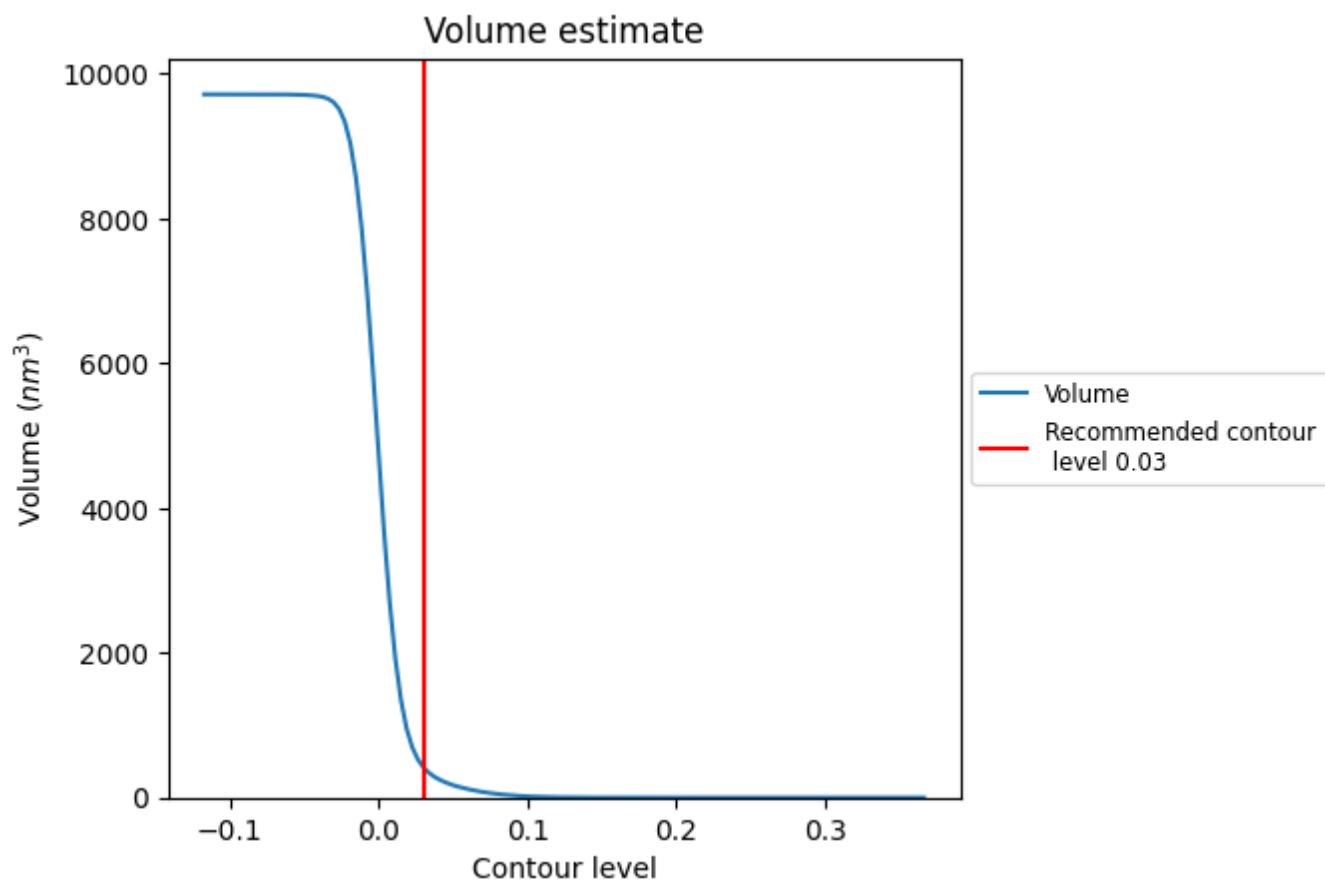
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 420 nm³; this corresponds to an approximate mass of 379 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

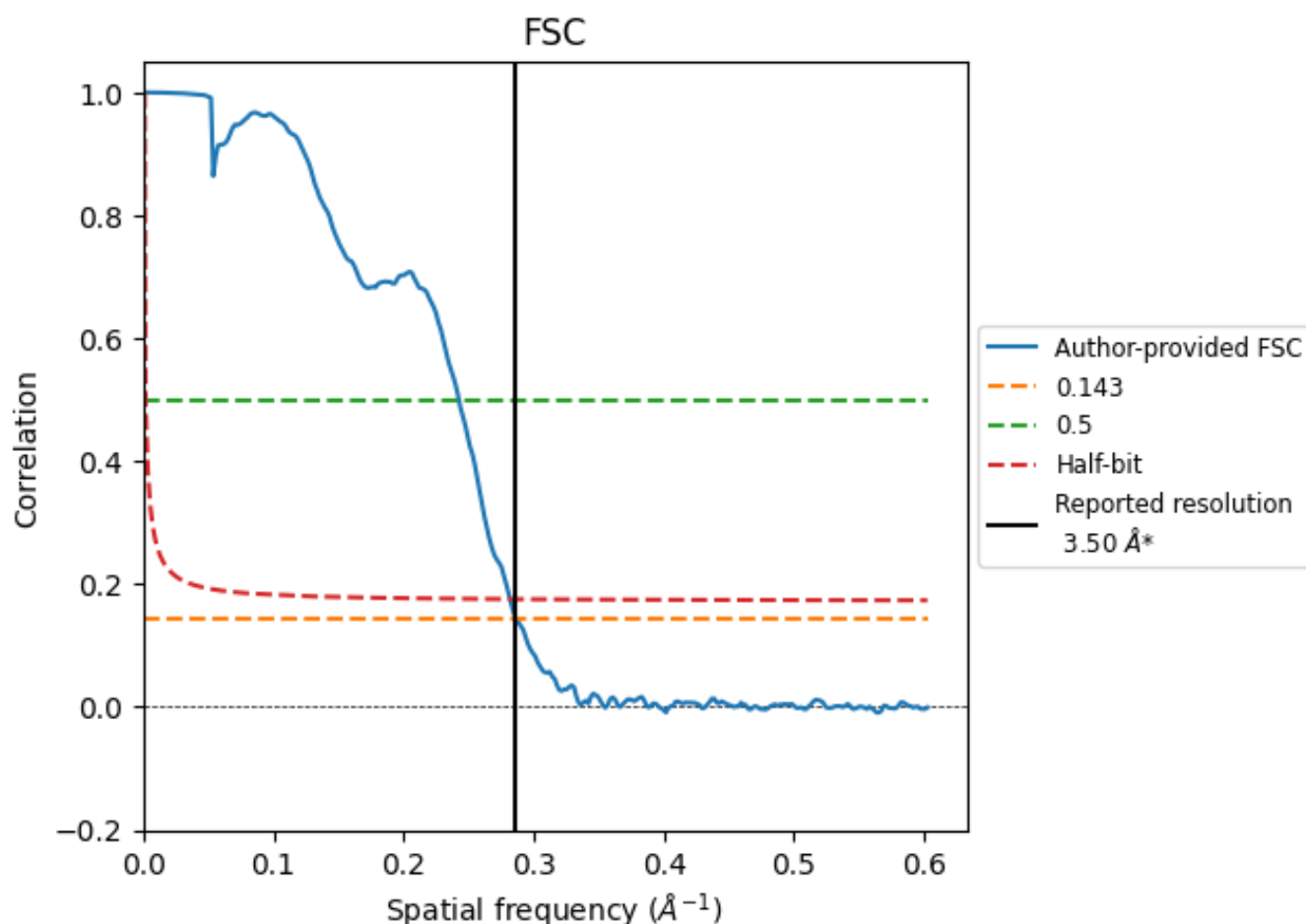
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.12	3.55
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

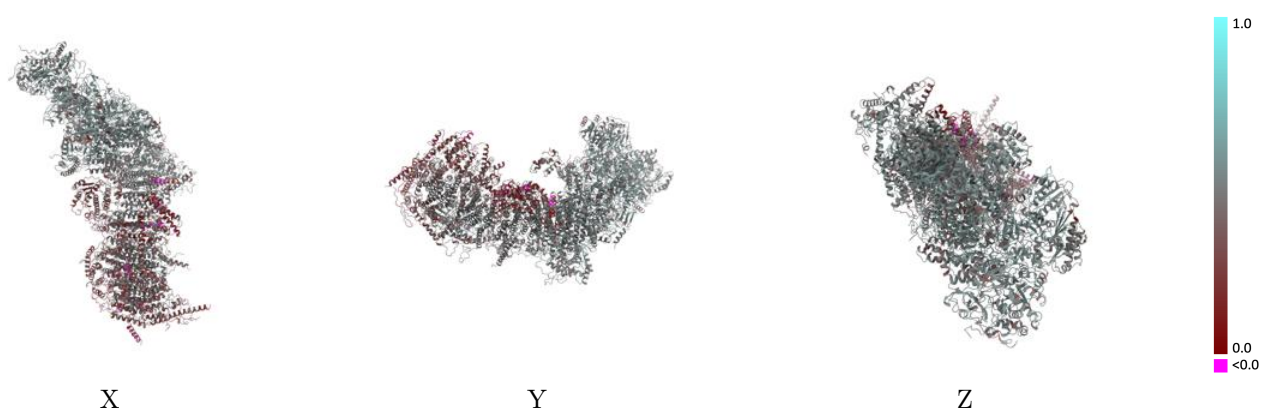
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11259 and PDB model 6ZKR. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

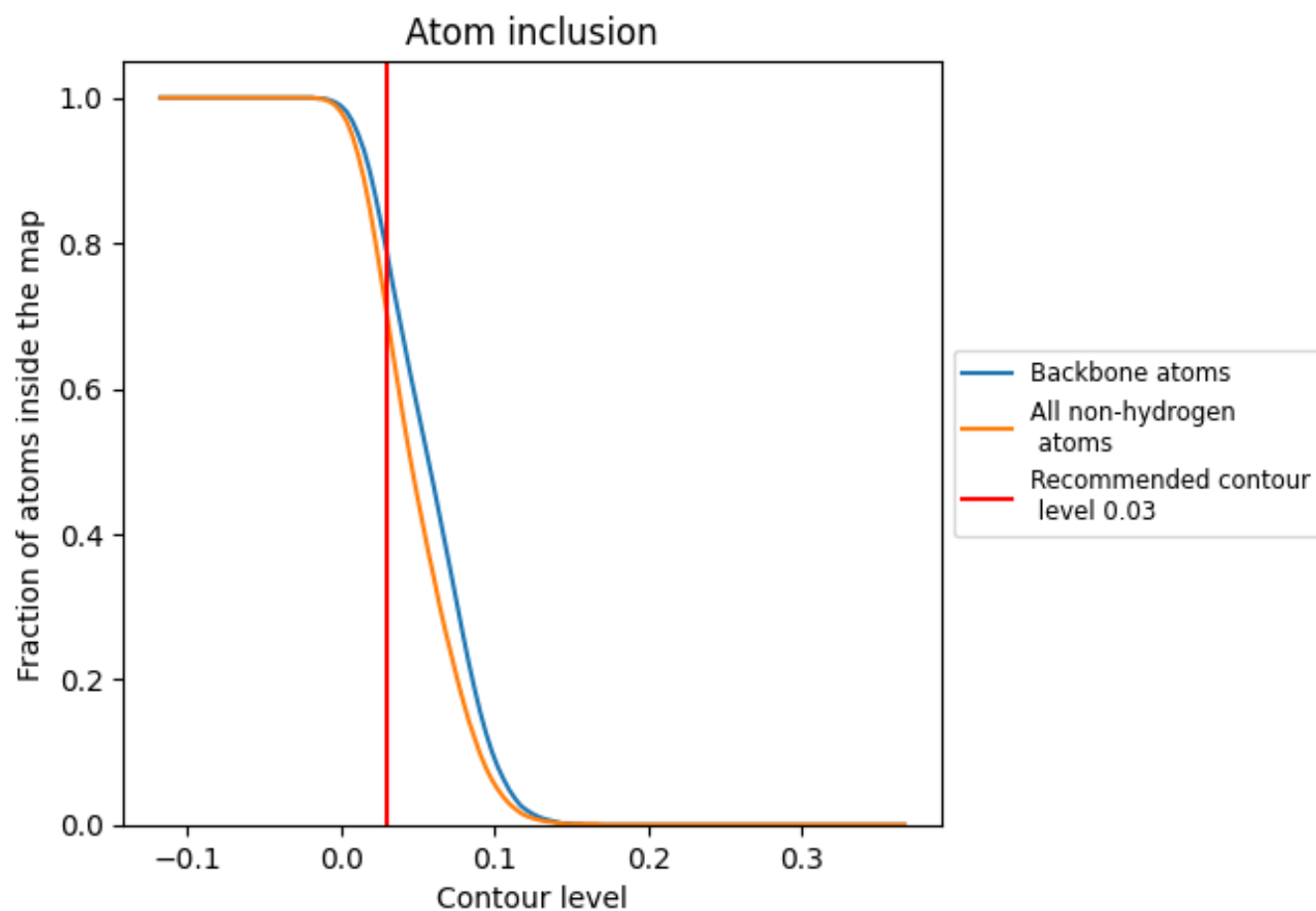


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7020	 0.4520
1	 0.8470	 0.5070
2	 0.8360	 0.4990
3	 0.8340	 0.5160
4	 0.7550	 0.5070
5	 0.8480	 0.5410
6	 0.8090	 0.5310
9	 0.8620	 0.5400
A	 0.6490	 0.4690
H	 0.7670	 0.5180
J	 0.6050	 0.4120
K	 0.6470	 0.4530
L	 0.5910	 0.3960
M	 0.6770	 0.4660
N	 0.6970	 0.4720
V	 0.1430	 0.2290
W	 0.7080	 0.4530
X	 0.5330	 0.2900
Y	 0.7570	 0.4790
Z	 0.7070	 0.4100
a	 0.8590	 0.4950
b	 0.8220	 0.5240
c	 0.8060	 0.5260
d	 0.8000	 0.4980
e	 0.8290	 0.4790
f	 0.7740	 0.4750
g	 0.7780	 0.4940
h	 0.8240	 0.5180
i	 0.8210	 0.5230
j	 0.6580	 0.3850
k	 0.3280	 0.3210
l	 0.7700	 0.4670
m	 0.8090	 0.5020
n	 0.5180	 0.2810
o	 0.6890	 0.4500



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Chain	Atom inclusion	Q-score
p	 0.5090	 0.3500
q	 0.7980	 0.4930
r	 0.6410	 0.3580
s	 0.6030	 0.3150
t	 0.5970	 0.3160
u	 0.6240	 0.3360
v	 0.5440	 0.3150
w	 0.6320	 0.4230
x	 0.6030	 0.3770
y	 0.6860	 0.4180
z	 0.8100	 0.5130